10511731

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LOGINID:SSPTANAG1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS	9	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS	10	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	11	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	12	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	13	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	14	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	15	DEC 18	CA/CAplus patent kind codes updated
NEWS	16	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS	17	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	18	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS	19	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals

NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:36:54 ON 11 JAN 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:37:03 ON 11 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 10 JAN 2007 HIGHEST RN 917201-58-2
DICTIONARY FILE UPDATES: 10 JAN 2007 HIGHEST RN 917201-58-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

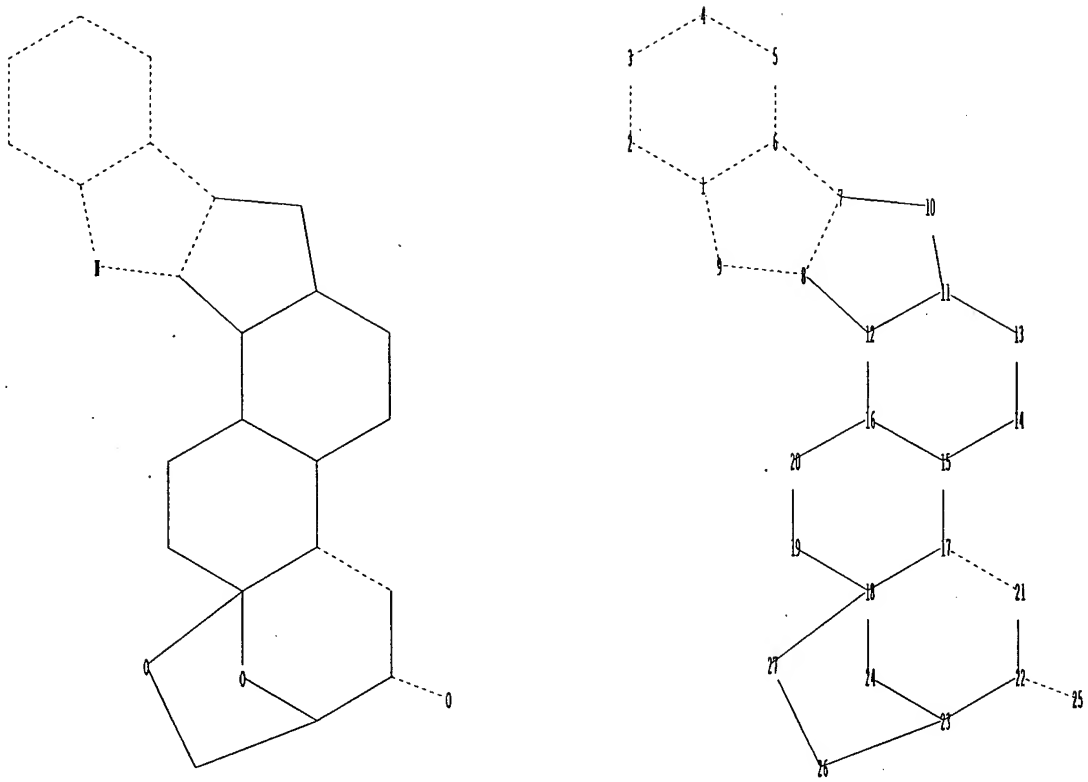
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10511731s1.str

10511731



chain nodes :
25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 26 27
chain bonds :
22-25
ring bonds :
1-2 1-6 1-9 2-3 3-4 4-5 5-6 6-7 7-8 7-10 8-9 8-12 10-11 11-12 11-13
12-16 13-14 14-15 15-16 15-17 16-20 17-18 17-21 18-19 18-24 18-27 19-20
21-22 22-23 23-24 23-26 26-27
exact/norm bonds :
1-2 1-6 1-9 2-3 3-4 4-5 5-6 6-7 7-8 7-10 8-9 8-12 10-11 11-12 11-13
12-16 13-14 14-15 15-16 15-17 16-20 17-18 17-21 18-19 18-24 18-27 19-20
21-22 22-23 22-25 23-24 23-26 26-27

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:Atom 27:Atom

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

10511731

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 17:37:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 106 TO 614
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 17:37:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 255 TO ITERATE

100.0% PROCESSED 255 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L3 13 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 172.31

FILE 'HCAPLUS' ENTERED AT 17:37:39 ON 11 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 11 Jan 2007 VOL 146 ISS 3
FILE LAST UPDATED: 10 Jan 2007 (20070110/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L4 62 L3

=> fil reg

10511731

'COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.60	174.91

FILE 'REGISTRY' ENTERED AT 17:38:27 ON 11 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 JAN 2007 HIGHEST RN 917201-58-2
DICTIONARY FILE UPDATES: 10 JAN 2007 HIGHEST RN 917201-58-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

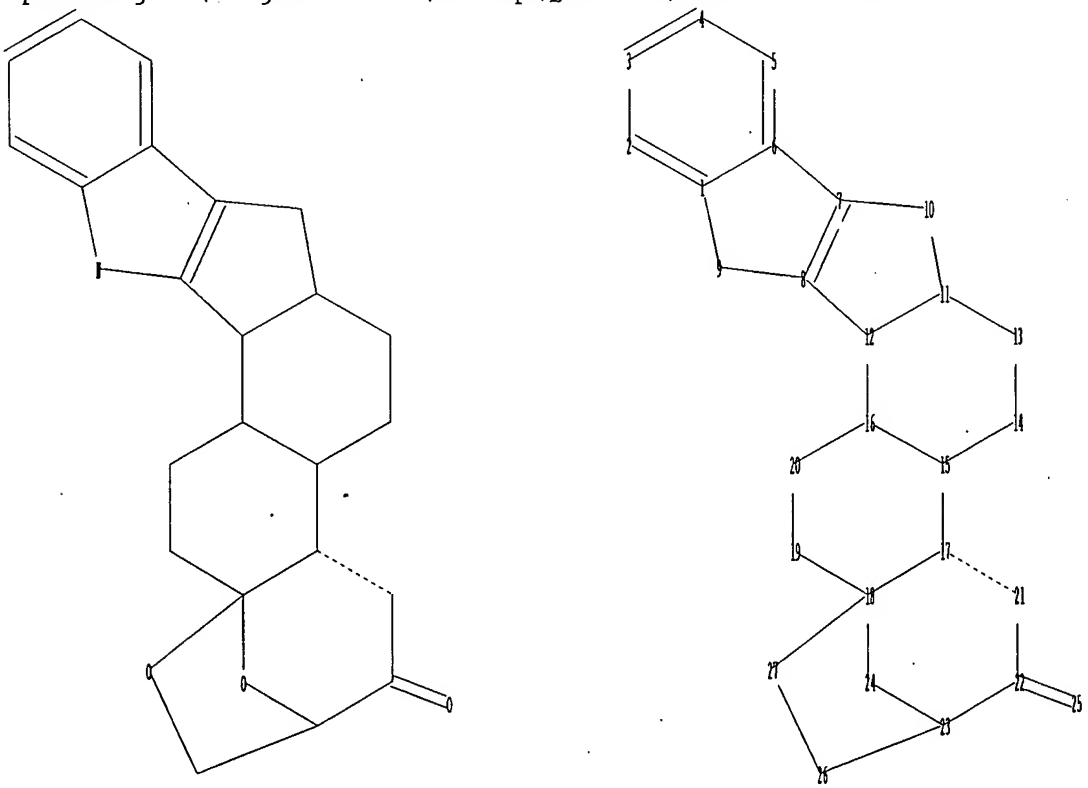
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10511731s2.str



chain nodes :

10511731

'25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 26 27
chain bonds :
22-25
ring bonds :
1-2 1-6 1-9 2-3 3-4 4-5 5-6 6-7 7-8 7-10 8-9 8-12 10-11 11-12 11-13
12-16 13-14 14-15 15-16 15-17 16-20 17-18 17-21 18-19 18-24 18-27 19-20
21-22 22-23 23-24 23-26 26-27
exact/norm bonds :
1-9 6-7 7-8 7-10 8-9 8-12 10-11 11-12 11-13 12-16 13-14 14-15 15-16
15-17 16-20 17-18 17-21 18-19 18-24 19-20 21-22 22-23 22-25 23-24
exact bonds :
18-27 23-26 26-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:Atom 27:Atom

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 17:40:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s lf ull
1136 LF
12 ULL
L7 0 LF ULL
(LF(W)ULL)

=> s l5 full

10511731

FULL SEARCH INITIATED 17:40:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS 12 ANSWERS
SEARCH TIME: 00.00.01

L8 12 SEA SSS FUL L5

=> fil hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	183.35	358.26

FILE 'HCAPLUS' ENTERED AT 17:40:45 ON 11 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 11 Jan 2007 VOL 146 ISS 3
FILE LAST UPDATED: 10 Jan 2007 (20070110/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8
L9 61 L8

=> d ed ibib abs hitstr 1-61

L9 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 03 Nov 2006
ACCESSION NUMBER: 2006:1156323 HCAPLUS
DOCUMENT NUMBER: 145:465702
TITLE: Immune response inhibition using indole diterpene compound
INVENTOR(S): Dalziel, Julie Eleanor; Dunlop, James; Finch, Sarah Christine; Wong, Shu Shyan
PATENT ASSIGNEE(S): Agresearch Limited, N. Z.
SOURCE: PCT Int. Appl., 51pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006115423	A1	20061102	WO 2006-NZ86	20060426

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

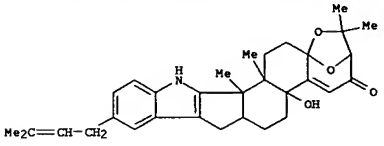
PRIORITY APPLN. INFO.: NZ 2005-538116 A 20050428

AB The invention relates to uses and methods of using indole diterpene compds. or derivs. thereof to influence the production of cytokines from cells and therefore influence an immune response. Applications are described including diagnosis methods, treatments for avoiding an undesirable immune response such as infection, sepsis, allergies, transplant rejection, and anaphylactic shock. Use in terms of pain prevention or reduction of inflammation is also described. Lolitrem B demonstrated immunosuppressant activity by inhibiting TNFα and IL-6 production in murine macrophages stimulated by lipopolysaccharide.

IT 11024-55-8, Paspalicine 11024-55-8D, Paspalicine, derivs.; isomers or analogs 63722-90-7, Paspalitrem A 63722-90-7D, Paspalitrem A, derivs.; isomers or analogs 63722-91-8, Paspalinine 63722-91-8D, Paspalinine, derivs.; isomers or analogs 63764-58-9, Paspalitrem B 63764-58-9D, Paspalitrem B, derivs.; isomers or analogs 90866-61-8, Paspalitrem C 90866-61-8D, Paspalitrem C, derivs.; isomers or analogs
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immune response inhibition using indole diterpene compound)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63722-91-8 HCAPLUS
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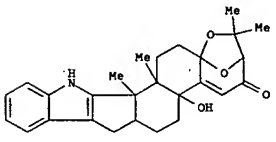

RN 63722-91-8 HCAPLUS
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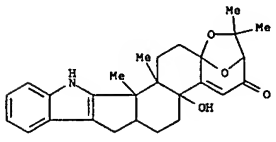
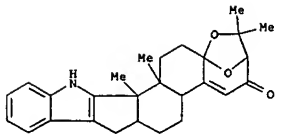
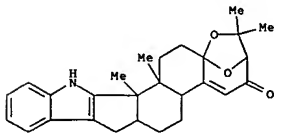


RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)-(9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



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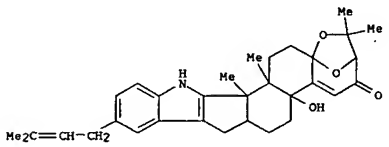

RN 63722-90-7 HCAPLUS
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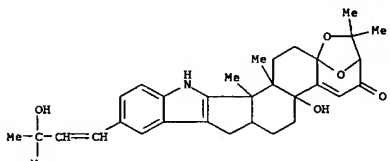
L9 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63764-58-9 HCAPLUS
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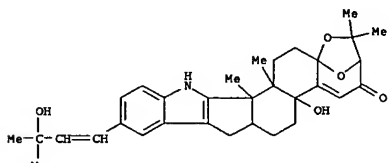

RN 90866-61-8 HCAPLUS
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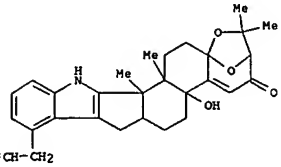

RN 90866-61-8 HCAPLUS
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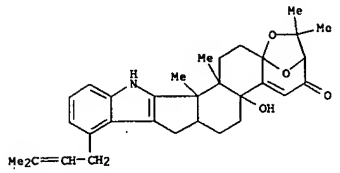
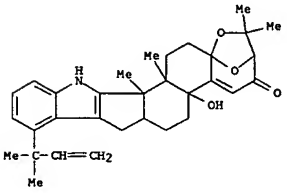
L9 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 30 Oct 2006
ACCESSION NUMBER: 2006:1127860 HCAPLUS
TITLE: Toxicology of tremorgenic mycotoxins on chicks
AUTHOR(S): Rafiyuddin, Md.; Rao, N. Janakirama; Girisham, S.; Reddy, S. M.
CORPORATE SOURCE: Department of Microbiology, Kakatiya University, Warangal, 506 009, India
SOURCE: National Academy Science Letters (India) (2006), 29(7 & 8), 311-315
CODEN: NASLDX; ISSN: 0250-541X
PUBLISHER: National Academy of Sciences, India
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Toxicity of aflatrem and penitrem A produced by Aspergillus flavus and Penicillium puberulum was tested on chicks. Significant decrease in iron, proteins, calcium, abumins and urea of serum, while increase in SGOT and SGPT was recorded under the influence of penitrem A. Similarly WBC decreased, while RBC increased due to penitrem A. Significant changes in proteins, glycogen, and cholesterol of liver, brain, heart and kidney were also recorded. Histopathol. changes of much significance were also recorded in tissues of heart, liver and brain.
IT INDEXING IN PROGRESS
IT 70553-75-2, Aflatrem
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(aflatrem and penitrem A produced by Aspergillus flavus and Penicillium puberulum tested on chicks)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



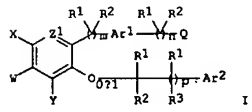
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 09 Dec 2005
ACCESSION NUMBER: 2005:1289303 HCAPLUS
DOCUMENT NUMBER: 144:36257
TITLE: Preparation of substituted benzoic acid and analogs as EP4 receptor agonists for treatment of glaucoma and related diseases
INVENTOR(S): Belley, Michel; Colucci, John; Girard, Mario; Han, Yongxin; Lacombe, Patrick
PATENT ASSIGNEE(S): Merck Frosst Canada Ltd., Can.
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

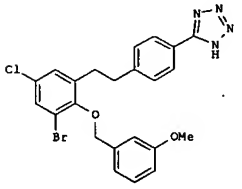
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005116010	A1	20051208	WO 2005-CA773	20050520
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2004-574653P P 20040526
OTHER SOURCE(S): MARPAT 144:36257
GI

L9 ANSWER 3 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

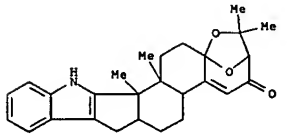


I



II

AB Title compds. I [Z1 = CW1, N; W1, X, W = H, amino, halo; Y = H, halo, alkoxy, etc.; R1-2 = H, halo, alkyl, etc.; R3 = R1, OH, etc.; Q = carboxy, tetrazolyl, etc.; Ar1 = Ph, pyridinyl, thienyl, etc.; Ar2 = benzoxadiazolyl, Ph, pyridyl, etc.] are prepared For instance, II is prepared in 4 steps from 3-bromo-5-chloro-2-hydroxybenzaldehyde, 3-methoxybenzyl bromide, 4-bromobenzonitrile and azidotributyltin. II has a binding affinity for the EP4 subtype of prostaglandin E2 receptor of 2.0 nM. I are useful for the treatment of glaucoma and other conditions which are related to elevated intraocular pressure in the eye of a patient. I are also used for mediating the bone modeling and remodeling processes of osteoblasts and osteoclasts.
IT 11024-55-8, Paspalicine
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(agonists of EP4 receptor subtype of PGE2 receptors and their use for treatment of glaucoma, other conditions and for mediating bone modeling and remodeling processes of osteoblasts and osteoclasts)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 3 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 14 Oct 2005
ACCESSION NUMBER: 2005:1106800 HCAPLUS
DOCUMENT NUMBER: 143:387049
TITLE: Preparation of disubstituted piperidinones, oxazinanones, thiazinanones, and morpholinones as EP4 receptor agonist for treatment of ocular and bone disorders
INVENTOR(S): Billot, Xavier; Colucci, John; Han, Yongxin; Wilson, Marie-claire; Young, Robert N.
PATENT ASSIGNEE(S): Can.
SOURCE: U.S. Pat. Appl. Publ., 30 pp., Division of U.S. Ser. No. 297,257.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

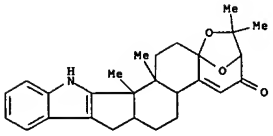
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005227969	A1	20051013	US 2005-146992	20050607
US 2004198701	A1	20041007	US 2004-797257	20040310
US 7053085	B2	20060530		
PRIORITY APPLN. INFO.:			US 2004-797257	A3 20040310
			US 2003-457700P	P 20030326

OTHER SOURCE(S): MARPAT 143:387049

AB This invention relates to potent selective agonists of the EP4 subtype of prostaglandin E2 receptors, their use or a formulation thereof in the treatment of glaucoma and other conditions, which are related to elevated intraocular pressure in the eye of a patient. This invention further relates to the use of the compds. of this invention for mediating the bone modeling and remodeling processes of the osteoblasts and osteoclasts. In particular, this invention relates to a series of 1,6-disubstituted piperidin-2-one, 3,4-disubstituted 1,3-oxazinan-2-one, 3,4-disubstituted 1,3-thiazinan-2-one, and 4,5-disubstituted morpholin-3-one derivs. The compds. of the invention are optionally formulated with other therapeutic agents useful in treating eye disorders or in stimulating bone formation such as β-adrenergic blocking agents, carbonic anhydrase inhibitors, and bisphosphonates. Preparation schemes for the compds. of the invention are disclosed.

IT 11024-55-8, Paspalicine
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(addnl. therapeutic agent; preparation of disubstituted piperidinones, oxazinanones, thiazinanones, and morpholinones as EP4 receptor agonists for treatment of ocular and bone disorders)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 4 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

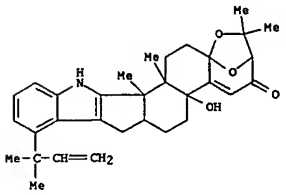


L9 ANSWER 5 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 22 Nov 2004
ACCESSION NUMBER: 2004:1000947 HCAPLUS
DOCUMENT NUMBER: 142:87348
TITLE: Indole-diterpene gene cluster from Aspergillus flavus
AUTHOR(S): Zhang, Shuguang; Monahan, Brendon J.; Tkacz, Jan S.; Scott, Barry
CORPORATE SOURCE: Centre for Functional Genomics, Institute of Molecular BioSciences, Massey University, Palmerston North, N. 2.
SOURCE: Applied and Environmental Microbiology (2004), 70(11), 6875-6883
CODEN: AEMIDF; ISSN: 0099-2240
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Aflatrem is a potent tremorgenic mycotoxin produced by the soil fungus Aspergillus flavus and is a member of a large structurally diverse group of secondary metabolites known as indole-diterpenes. By using degenerate primers for conserved domains of fungal geranylgeranyl diphosphate synthases, we cloned two genes, atmG and ggsA (an apparent pseudogene), from A. flavus. Adjacent to atmG are two other genes, atmC and atmM. These three genes have 64 to 70% amino acid sequence similarity and conserved synteny with a cluster of orthologous genes, paxG, paxC, and paxM, from Penicillium paxilli which are required for indole-diterpene biosynthesis. AtmG, atmC, and atmM are coordinately expressed, with transcript levels dramatically increasing at the onset of aflatrem biosynthesis. A genomic copy of atmM can complement a paxM deletion mutant of P. paxilli, demonstrating that atmM is a functional homolog of paxM. Thus, atmG, atmC, and atmM are necessary, but not sufficient, for aflatrem biosynthesis by A. flavus. This provides the first genetic evidence for the biosynthetic pathway of aflatrem in A. flavus.

IT 70553-75-2, Aflatrem
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(indole-diterpene gene cluster from Aspergillus flavus)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 May 2004
ACCESSION NUMBER: 2004:370925 HCAPLUS
DOCUMENT NUMBER: 140:391155
TITLE: A preparation of pyrrolidin-2-one derivatives as EP4 receptor agonists
INVENTOR(S): Billot, Zavier; Han, Yongxin; Young, Robert N.; Girard, Mario; Wilson, Marie-Claire
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.; Beunard, Jean-Luc; Colucci, John
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

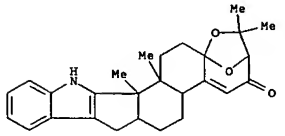
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037813	A1	20040506	WO 2003-CA1618	20031023
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003275838	A1	20040513	AU 2003-275838	20031023
PRIORITY APPLN. INFO.:			US 2002-421503P	P 20021025
			WO 2003-CA1618	W 20031023

OTHER SOURCE(S): MARPAT 140:391155
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to pyrrolidin-2-one derivs. of formula I [wherein: Y is C(O) or CH(OH); Y1 = (CH2)2, CH:CH, or 1,2-cyclopropanediyl; Z = O, S, 1,2-cyclopropanediyl, CH:CH, C.tplbond.C, or a bond; R1 = CHO, OH, CN, etc.; Q is a divalent (hetero)arylene group; W is a bond, CH:CH, unsubstituted C1-6 alkylene, or a C1-6 alkylene substituted with 1-4 halogen atoms; R2 = C1-6alkyl, (CH2)0-8-C6-10aryl, O-C3-10cycloalkyl, O-C1-10alkyl, etc.], useful as selective agonists of the EP4 subtype of prostaglandin E2 receptors. The invention compds. are useful for the treatment of glaucoma and other conditions which are related to elevated intraocular pressure in the eye of a patient. The invention relates to the use of the title compds. for mediating the bone modeling and remodeling processes of the osteoblasts and osteoclasts. The effect of the prepared EP4 agonist compds. on intraocular pressure in rabbits and monkeys was investigated. The compds. were also tested in bone resorption assays (EC50 = 0.001-100 μM). For instance, compound II was prepared via amination of cinnamate derivative III by pyrrolidine derivative IV, hydrolysis of

L9 ANSWER 6 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
the obtained pyrrolidine deriv. V (R3 = OMe, R4 = CH2OTBDMS), addn. of BnC(O)CH2P(O)(OEt)2, redn. of the obtained unsatd. ketone V [R3 = OMe, R4 = CH:CHC(O)Bn], and subsequent hydrolysis (example 1, no yield data).
IT 11024-55-8, Paspalicine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Maxi-K channel blocker, drug component; preparation of pyrrolidin-2-one derivs. as EP4 receptor agonists)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 7 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 May 2004
ACCESSION NUMBER: 2004:370901 HCAPLUS
DOCUMENT NUMBER: 140:391154
TITLE: A preparation of pyrrolidinone derivatives useful as selective EP4 receptor agonists
INVENTOR(S): Billot, Xavier; Beunard, Jean-Luc; Han, Yongxin; Young, Robert N.; Colucci, John; Girard, Mario; Wilson, Marie-Claire
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

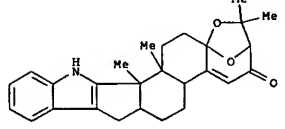
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037786	A2	20040506	WO 2003-CA1620	20031023
WO 2004037786	A3	20040930		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2502914	A1	20040506	CA 2003-2502914	20031023
AU 2003275840	A1	20040513	AU 2003-275840	20031023
EP 1558602	A2	20050803	EP 2003-809227	20031023
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006505572	T	20060216	JP 2004-545645	20031023
US 2006167081	A1	20060727	US 2005-528419	20050317
PRIORITY APPLN. INFO.:			US 2002-421402P	P 20021025
			WO 2003-CA1620	W 20031023

OTHER SOURCE(S): MARPAT 140:391154
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to pyrrolidinone derivs. of formula I [wherein: Y1 = (CH2)2, CH:CH, 1,2-cyclopropanediyl; Y is C(O) or CH(OH); A is (CH2)1-4; Z = O, S, 1,2-cyclopropanediyl, HC:CH, C.tplbond.C, or a bond; Q is a disubstituted (hetero)aryl ring; W is a bond, unsubstituted C1-6 alkylene, or C1-6 alkylene substituted with 1-4 halogen atoms; R1 = OH, CN, CHO, etc.; R2 = C1-6alkyl, (CH2)0-8-(C6-10aryl), O-C1-10alkyl, etc.; R3 and R4 are independently selected from halogen, C1-6alkyl, or R3 and R4, together with the carbon atom to which they are attached, form a C3-7 cycloalkyl ring] useful as potent selective agonists of the EP4 subtype of prostaglandin E2 receptors. The invention compds. are useful in treatment of glaucoma and other conditions which are related to the elevated intraocular pressure in the eye. The invention relates to the use of the invention compds. for mediating the bone modeling and remodeling processes

L9 ANSWER 7 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
of the osteoblasts and osteoclasts. The invention compds. were tested as EP4 agonists on intraocular pressure in rabbits and monkeys; prostanoid receptor binding assays and bone resorption assays were performed (in a subclass of the invented compds., agonists have EC50 values from 0.01 μM to 10 μM). The synthesized stereoisomeric pyrrolidinones II were prepd. from pyrrole deriv. III via oxidn., condensation with PhCF2C(O)CH2P(O)(OMe)2, keto-group redn. of the obtained unsatd. ketone IV, alc. protection, N-cleavage, addn. of thiophene deriv. V to the obtained compd. VI, sepn. of the isomers, alc. deprotection, and hydrolysis.
IT 11024-55-8, Paspalicine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Maxi-K channel blocker, drug component; preparation of pyrrolidinone derivs. useful as selective EP4 receptor agonists)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

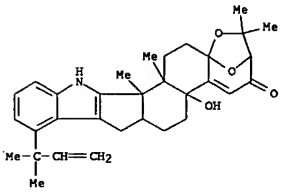


L9 ANSWER 8 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 Dec 2003
ACCESSION NUMBER: 2003:1014246 HCAPLUS
DOCUMENT NUMBER: 140:339503
TITLE: Tremorgenic and nontremorgenic 2,3-fused indole diterpenoids
AUTHOR(S): Sings, Heather; Singh, Sheo
CORPORATE SOURCE: Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Alkaloids (San Diego, CA, United States) (2003), 60, 51-163
CODEN: ALKAAR; ISSN: 0099-9598
PUBLISHER: Elsevier Science
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review of synthesis, natural origin, properties and tremorgenic activity of diterpenoid indole alkaloids was presented. The diterpenoid alkaloids reviewed were divided into groups which included paspalanes, aflatremanes, penitremanes, janthitremanes, and lolitremanes. The reported biol. activities of some of these alkaloids have included definitions of various tremors and staggers, which were reviewed in 1989, including a proposal for a pharmacophore model for γ-aminobutyric acid (GABA) activity. Also included were details of the isolation and structure elucidation, chemical modifications, and biol. activities of all alkaloids reported in the published literature until 2002.

IT 70553-75-2DP, Aflatrem, analogs
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(natural origin, properties and synthesis of tremorgenic and nontremorgenic 2,3-fused indole diterpenoids)

RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 165 THERE ARE 165 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 26 Dec 2003
ACCESSION NUMBER: 2003:1006788 HCAPLUS
DOCUMENT NUMBER: 140:53461
TITLE: Maxi-K potassium channel blockers for treatment of glaucoma and as ocular neuroprotective agents
INVENTOR(S): Goetz, Michael A.; Kaczorowski, Gregory J.; Monaghan, Richard L.; Strohl, William R.; Tkacz, Jan S.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

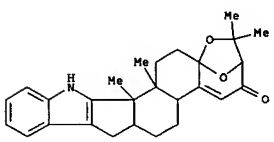
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003105868	A1	20031224	WO 2003-US19013	20030613
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2488884	A1	20031224	CA 2003-2488884	20030613
AU 2003245531	A1	20031231	AU 2003-245531	20030613
EP 1515730	A1	20050323	EP 2003-739159	20030613
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005538061	T	20051215	JP 2004-512770	20030613
US 2005239787	A1	20051027	US 2004-511664	20041018
PRIORITY APPLN. INFO.:			US 2002-389205P P	20020617
			WO 2003-US19013 W	20030613

AB The invention discloses the use of potent potassium channel blockers or a formulation thereof in the treatment of glaucoma and other conditions related to elevated intraocular pressure in the eye of a patient. The invention also discloses the use of such compds. to provide a neuroprotective effect to the eye of a mammalian species, particularly humans.

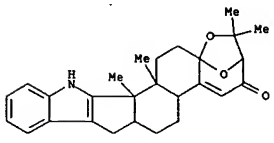
IT 11024-55-8, Paspalicine 11024-55-8D, Paspalicine, enantiomers and diastereomers 63722-90-7, Paspalitrem a 63722-90-7D, Paspalitrem a, enantiomers and diastereomers 63722-91-8, Paspalinine 63722-91-8D, Paspalinine, enantiomers and diastereomers 63764-58-9, Paspalitrem b 63764-58-9D, Paspalitrem b, enantiomers and diastereomers 90866-61-8, Paspalitrem c 90866-61-8D, Paspalitrem c, enantiomers and diastereomers
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(maxi-K potassium channel blockers for treatment of glaucoma and as ocular neuroprotective agents)

RN 11024-55-8 HCAPLUS

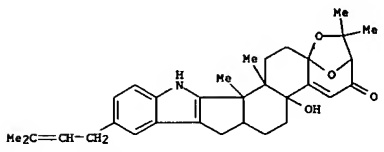
L9 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

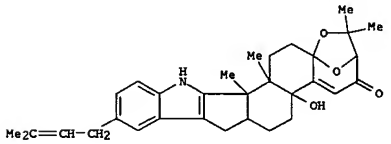


RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

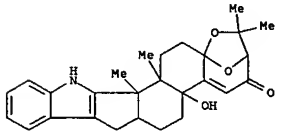


RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

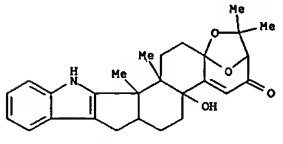
L9 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

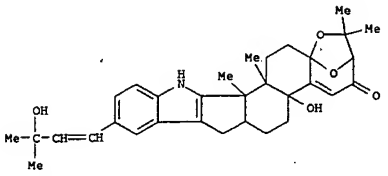


RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

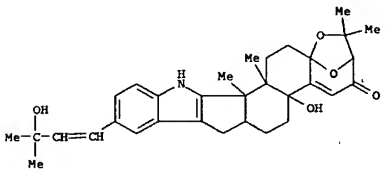


RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

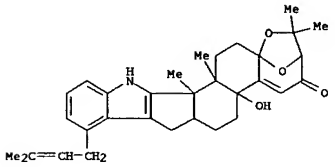
L9 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



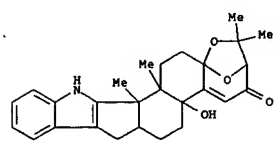
RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)-(9CI) (CA INDEX NAME)



RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



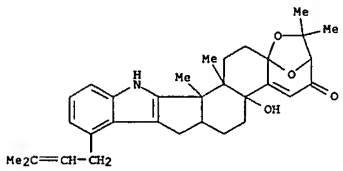
L9 ANSWER 10 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 16 Jun 2003
ACCESSION NUMBER: 2003:459324 HCAPLUS
DOCUMENT NUMBER: 140:106640
TITLE: Fungal metabolite screening: database of 474 mycotoxins and fungal metabolites for dereplication by standardized liquid chromatography-UV-mass spectrometry methodology
AUTHOR(S): Nielsen, Kristian Fog; Smedsgaard, Jorn
CORPORATE SOURCE: BioCentrum-DTU, Mycology Group, Technical University of Denmark, Lyngby, DK-2800, Den.
SOURCE: Journal of Chromatography, A (2003), 1002(1-2), 111-136
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A standardized LC-UV-MS micro-scale method for screening of fungal metabolites and mycotoxins in culture exts. is presented. The paper includes data for detection and dereplication of >400 fungal metabolites to facilitate detection and identification when stds. are not available. The data also shows the types of components that can be analyzed by pos. electrospray (ESI+) mass spectrometry (MS) along with common fragments and adducts of these, as well as giving suggestions on whether UV or ESI+-MS methods should be used. Examples of dereplication of penitrems and macro-cyclic trichothecenes, and detection of several novel compds. are shown. This was done by UV spectroscopy combined with accurate mass determination of adduct and fragment ions obtained by high-resolution orthogonal time-of-flight MS.
IT 63722-91-8, Paspalinin 70553-75-2, Aflatrem
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(database of 474 mycotoxins and fungal metabolites for dereplication by standardized liquid chromatog.-UV-mass spectrometry methodol.)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

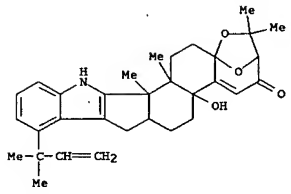
L9 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



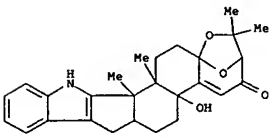
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 10 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



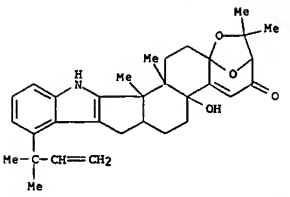
REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Feb 2002
ACCESSION NUMBER: 2002:127616 HCAPLUS
DOCUMENT NUMBER: 136:305407
TITLE: Toxigenic fungi in human environment
AUTHOR(S): Krikstaponis, A.; Stakeniene, J.; Lugauskas, A.
CORPORATE SOURCE: Institute of Botany, Vilnius, LT-2021, Lithuania
SOURCE: Biologija (2001), (4), 10-12
CODEN: BOLOE8; ISSN: 1392-0146
PUBLISHER: Lietuvos Mokslu Akademijos Leidykla
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Fungal species compns. on vegetable-born food products and in the air and dust of dwellings were studied in 1996-2000. Seven food selling-storage places and 14 residences were investigated, 179 samples of 94 names of food products as well as 50 air and 110 dust samples were surveyed. Ability of 393 fungal isolates to produce secondary metabolites grown on Czapek - yeast extract and yeast extract - sucrose agar media was tested, 124
strains were regarded as active producers of secondary metabolities.
IT 63722-91-8, Paspalinin 70553-75-2, Aflatrem
RL: POL (Pollutant); OCCU (Occurrence)
(toxigenic fungi in human environment)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



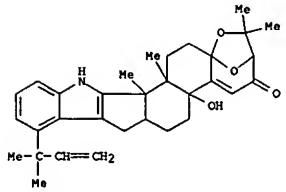
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 11 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 12 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 13 Jan 2000
ACCESSION NUMBER: 2000:28384 HCAPLUS
DOCUMENT NUMBER: 132:307469
TITLE: Mycoflora and mycotoxins of Brazilian cashew kernels
AUTHOR(S): Freire, Francisco C. O.; Kozakiewicz, Zofia; Paterson, R. Russell M.
CORPORATE SOURCE: Centro Nacional de Pesquisa de Agroindustria Tropical, Ceara, Brazil
SOURCE: Mycopathologia (1999), 145(2), 95-103
CODEN: MYCPAH; ISSN: 0301-486X
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Kernel samples of common and dwarf Brazilian cashew nuts were highly contaminated with field and storage fungi in comparison to healthy ones. In general, dwarf cashews were more contaminated than common. A total of 37 fungal species were identified. Aspergillus niger was the dominant species with more colonies being isolated from dwarf kernels. A. flavus was the next most frequently isolated species. Penicillium brevicompactum, and P. glabrum were the most frequently isolated penicillia, with higher contamination recorded from dwarf kernels. Chaetomium globosum was recorded at a high level. Nine species were recorded from cashew kernels for the 1st time. Multimycotoxin anal. by TLC and HPLC were pos. for mycotoxins and other secondary metabolites particularly from the infected samples. HPLC was only carried out on dwarf cashews. Aflatoxins were not detected by quant. high performance thin layer chromatog.
IT 70553-75-2, Aflatrem
RL: POL (Pollutant); OCCU (Occurrence)
(mycoflora and mycotoxins of Brazilian cashew kernels)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

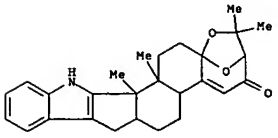


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 13 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Jul 1999
ACCESSION NUMBER: 1999:450819 HCAPLUS
DOCUMENT NUMBER: 131:97619
TITLE: Method for reducing intraocular pressure in the mammalian eye by administration of potassium channel blockers
INVENTOR(S): Adorante, Joseph S.; Woldemussie, Elizabeth; Ruiz, Guadalupe; Kopper, Kara; Moore, Alison M.
PATENT ASSIGNEE(S): Allergan, USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5925342	A	19990720	US 1997-891623	19970709
PRIORITY APPLN. INFO.:			US 1996-748671	A1 19961113

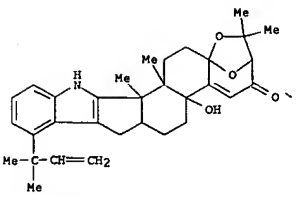
AB Pharmaceutical compns. and a method are disclosed for treating glaucoma and/or ocular hypertension in the mammalian eye by administering to the mammalian eye the pharmaceutical composition of the invention which contains,
as the active ingredient, one or more compds. having potassium channel blocking activity. Examples of potassium channel blockers utilized in the pharmaceutical composition and method of treatment are quinine, tremogenic indole alkaloids, such as Penitrem A and paspalicine, and insect toxins such as charybdotoxin and iberiotoxin. Quinine was tested in rabbit eyes and in bovine nonpigmented ciliary epithelial cells.
IT 11024-55-8, Paspalicine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(as potassium channel blocker; potassium channel blockers for reducing intraocular pressure in mammalian eye)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

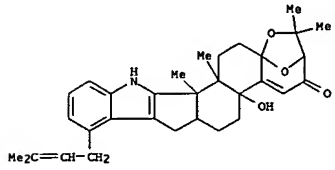
L9 ANSWER 14 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 01 May 1998
ACCESSION NUMBER: 1998:247492 HCAPLUS
DOCUMENT NUMBER: 129:14059
TITLE: Liquid chromatographic determination of major secondary metabolites produced by Aspergillus species from section Flavi
AUTHOR(S): Sobolev, Victor S.; Horn, Bruce W.; Dorner, Joe W.; Cole, Richard J.
CORPORATE SOURCE: Agric. Res. Service, Natl. Peanut Res. Lab., U.S. Dep. Agric., Dawson, GA, 31742, USA
SOURCE: Journal of AOAC International (1998), 81(1), 57-60
CODEN: JAINEE; ISSN: 1060-3271
PUBLISHER: AOAC International, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A liquid chromatog. (LC) method was developed for simultaneous determination of major secondary metabolites - including cyclopiazonic acid (CPA), O-methylsterigmatocystin (OMST), and the versicolorins - produced by Aspergillus species from section Flavi (A. flavus, A. parasiticus, A. tamarii, and A. caelatus) on a liquid medium. Metabolites were extracted with chloroform and quantitated without prior cleanup by means of normal-phase ion-pair partition LC on silica gel with a mobile phase of n-heptane-2-propanol-n-butanol-water-tetrabutylammonium hydroxide (2560+900 + 230+32 + 8, volume/volume). Recoveries of CPA and OMST from fungal cultures spiked at 10 μg/mL were 98.90±3.27 and 95.92±5.27% (n=5), resp. At spike levels of 100 μg/mL, recoveries were 98.89±3.87 and 97.65±4.32% (n=5), resp. Limits of detection for pure stds. were 0.25 μg/mL for CPA (at 280 nm) and 0.30 μg/mL for OMST (at 310 nm). UV detector responses to CPA and OMST were linear to about 0.5 and 3.5 μg/injection, resp.
IT 70553-75-2, Aflatrem
RL: ANT (Analyte); ANST (Analytical study)
(liquid chromatog. determination of major secondary metabolites produced by Aspergillus species from section Flavi)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 14 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 15 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 26 Dec 1996
ACCESSION NUMBER: 1996:756504 HCAPLUS
DOCUMENT NUMBER: 126:26785
TITLE: Effects of the K+ channel blockers paspalitrem-C and paxilline on mammalian smooth muscle
AUTHOR(S): DeFarias, Fernando P.; Carvalho, Marcia F.; Lee, Seok H.; Kaczorowski, Gregory J.; Suarez-Kurtz, Guilherme
CORPORATE SOURCE: Dep. Bioquim. Med., Univ. Fed. Rio de Janeiro, Rio de Janeiro, RJ-21941-590, Brazil
SOURCE: European Journal of Pharmacology (1996), 314(1/2), 123-128
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The tremorgenic alkaloids, paxilline and paspalitrem-C (0.1-10 μM), increased the spontaneous contractility of guinea-pig and rat urinary bladder, and rat duodenum, and induced tension in guinea-pig trachea. These effects are ascribed to blockade of high-conductance, Ca2+-activated K+ (BKCa) channels. Paxilline potentiated the charybdotoxin-induced stimulation of guinea-pig detrusor muscle; this is consistent with the alkaloid's ability to allosterically enhance the binding of charybdotoxin to smooth muscle membranes (Knaus et al., 1994). Paspalitrem-C and paxilline did not affect the myogenic activity of isolated portal vein from guinea-pig, which is insensitive to charybdotoxin, or of that from rat which is stimulated by charybdotoxin. Paxilline and paspalitrem-C also differed from charybdotoxin in that the alkaloids did not consistently elicit tension in guinea-pig aortic rings. These discrepancies are attributed to differences in relative potency, sites and/or mechanisms of action of the indole alkaloids vs. peptidyl blockers of the BKca channel.
IT 90866-61-8, Paspalitrem-C
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effects of K+ channel blockers paspalitrem-C and paxilline on mammalian smooth muscle)
RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



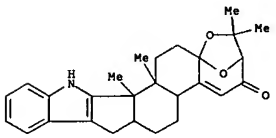
L9 ANSWER 16 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 27 Nov 1996
ACCESSION NUMBER: 1996:701991 HCAPLUS
DOCUMENT NUMBER: 126:1219
TITLE: Method for reducing intraocular pressure in the mammalian eye by administration of potassium channel blockers
INVENTOR(S): Adorante, Joseph S.; Woldemussie, Elizabeth; Ruiz, Guadalupe
PATENT ASSIGNEE(S): Allergan, USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5573758	A	19961112	US 1995-431170	19950428
CA 2219280	A1	19961031	CA 1996-2219280	19960416
WO 9633719	A1	19961031	WO 1996-US5241	19960416
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9655488	A	19961118	AU 1996-55488	19960416
AU 703241	B2	19990325		
EP 825863	A1	19980304	EP 1996-912798	19960416
EP 825863	B1	20021009		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11504330	T	19990420	JP 1996-532585	19960416
EP 1243270	A1	20020925	EP 2002-9867	19960416
EP 1243270	B1	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 225658	T	20021015	AT 1996-912798	19960416
ES 2182973	T3	20030316	ES 1996-912798	19960416
AT 251458	T	20031015	AT 2002-9867	19960416
ES 2204879	T3	20040501	ES 2002-9867	19960416

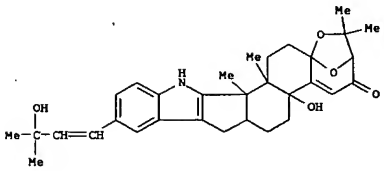
PRIORITY APPLN. INFO.: US 1995-431170 A 19950428
EP 1996-912798 A3 19960416
WO 1996-US5241 W 19960416

AB Pharmaceutical compns. and a method are disclosed for treating glaucoma and/or ocular hypertension in the mammalian eye by administering to the mammalian eye the pharmaceutical composition of the invention which contains, as the active ingredient, one or more compds. having potassium channel blocking activity. Examples of potassium channel blockers utilized in the pharmaceutical composition are quinine, tremogenic indole alkaloids, such as Penitrem A and paspalicine, and insect toxins such as charybdotoxin and iberiotoxin. In the in vivo studies normotensive rabbits were injected intracamerally with 1 mM quinine, resulting in IOP decrease by 7 mmHg and IOP remained depressed for 24 h.
IT 11024-55-8, Paspalicine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(potassium channel blockers for reducing intraocular pressure)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-,

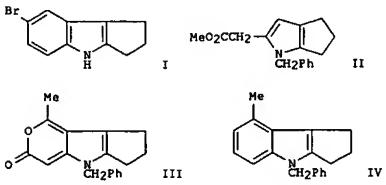
L9 ANSWER 16 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 17 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

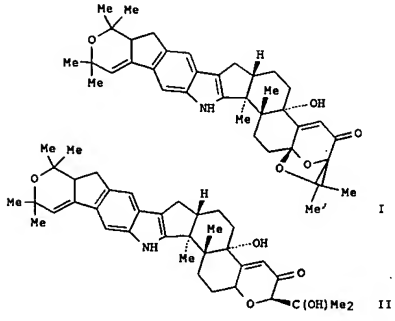


L9 ANSWER 17 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 May 1995
ACCESSION NUMBER: 1995:560774 HCAPLUS
DOCUMENT NUMBER: 123:56337
TITLE: Cyclopenta[b]indoles. Part 2. Model studies towards the tremorgenic mycotoxins
AUTHOR(S): Harrison, Carrie-Ann; Jackson, P. Mark; Moody, Christopher J.; Williams, Jonathan M. J.
CORPORATE SOURCE: Dep. of Chemistry, Loughborough Univ. of Technology, Leicestershire, LE11 3TU, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1995), (9), 1131-6
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:56337
GI



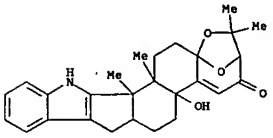
AB The 7-bromocyclopenta[b]indole I has been converted into the hydroxybutenyl derivs. and a tetrahydrofuranylidene derivative in model studies towards the elaboration of paspalitrem and lolitrem type side chains. In a parallel approach, the cyclopentapyrrole II was converted into the fused α-pyrone III which acted as a pyrrole-2,3-quinodimethane, and underwent Diels-Alder reaction to give, after loss of carbon dioxide, the cyclopentaindoles, e.g. IV.
IT 63764-58-9P, Paspalitrem B
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of cyclopentaindoles in model studies towards the tremorgenic
mycotoxins)
RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 18 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 1995
ACCESSION NUMBER: 1995:505350 HCAPLUS
DOCUMENT NUMBER: 122:286198
TITLE: Antiinsectan alkaloids: shearinines A-C and a new paxilline derivative from the ascostromata of Eupenicillium shearii
AUTHOR(S): Belofsky, Gilbert N.; Gloer, James B.; Wicklow, Donald T.; Dowd, Patrick F.
CORPORATE SOURCE: Dep. Chemistry, Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Tetrahedron (1995), 51(14), 3959-68
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

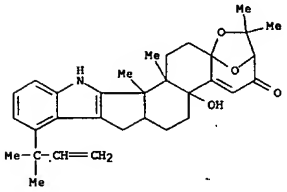


AB Four new antiinsectan indole alkaloids were isolated from organic exts. of the sclerotioid ascostromata of E. shearii (NRRL 3324). These exts. also afforded paxilline and 4 known, paxilline-related metabolites. The structures of the new compds. were determined through anal. of 1H NMR, 13C NMR,
HMQC, and HMBC expts. The 9 compds. were isolated from fractions displaying activity in dietary assays against the corn earworm Helicovepa zea and the dried-fruit beetle Carpophilus hemipterus, and most of the compds. show potent activity in these assays. Shearinine A (I) also exhibited activity in a topical assay against H. zea, and shearinine B (II) caused significant mortality in a leaf disk assay against the fall armyworm Spodoptera frugiperda.
IT 63722-91-8, Paspalinine
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(paxilline derivs. from the ascostromata of Eupenicillium shearii)
RN 63722-91-8 HCAPLUS

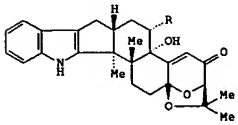
L9 ANSWER 18 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 19 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 Mar 1995
ACCESSION NUMBER: 1995:395485 HCAPLUS
DOCUMENT NUMBER: 122:290741
TITLE: Partial structures of the fungal toxin aflatrem, methyl-substituted 6,8-dioxabicyclo[3.2.1]octan-2-ones having anticonvulsant activity
AUTHOR(S): Tinao-Wooldridge, Luzviminda V.; Hsiang, Bonnie C. H.; Latifi, Tammy N.; Ferrendelli, James A.; Covey, Douglas F.
CORPORATE SOURCE: Dep. Mol. Biol. Pharmacology, Washington Univ. School Medicine, St. Louis, MO, 63110, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1995), 5(3), 265-70
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:290741
AB 4,7,7-Trimethyl-6,8-dioxabicyclo[3.2.1]octan-2-one was found to be an effective anticonvulsant (ED50 = 131 mg/kg) against pentylenetetrazole-induced seizures in mice. Enantioselectively was observed in the actions of the (+)- and (-)-enantiomers as anticonvulsants and as displacers of [35S]-TPBS, a ligand for the picrotoxin site on GABAA receptors. The (-)-enantiomer was slightly more potent in both biol. assays.
IT 70553-75-2DP, Aflatrem, partial structure derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(partial structures of fungal toxin aflatrem, methyl-substituted dioxabicyclooctanones having anticonvulsant activity)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

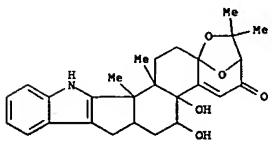


L9 ANSWER 20 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Jun 1994
ACCESSION NUMBER: 1994:293633 HCAPLUS
DOCUMENT NUMBER: 120:293633
TITLE: New paspalinine derivatives with antiinsectan activity from the sclerotia of Aspergillus nomius
AUTHOR(S): Staub, Gail M.; Gloer, Katherine B.; Gloer, James B.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Tetrahedron Letters (1993), 34(16), 2569-72
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



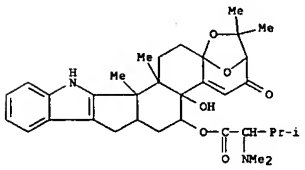
I, R=OH
II, R=O2CCH(NMe2)CHMe2

AB 14-Hydroxypaspalinine (I) and 14-(N,N-dimethyl-L-valyloxy)paspalinine (II) were isolated from the sclerotia of Aspergillus nomius, and identified by anal. of 2D NMR data. Both compds. caused 90% reduction in weight gain in assays against the corn earworm Helicoverpa zea at the 100 ppm (dry weight) dietary level. Paspalinine caused no effect at this concentration
IT 151341-77-4 151341-78-5
RL: PROC (Process)
(structure and isolation of, from Aspergillus nomius sclerotia, insecticidal activity in relation to)
RN 151341-77-4 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b,6-dihydroxy-2,2,13b,13c-tetramethyl-, [3R-(3a,5bα,6α,7aβ,13bα,13c.bet a.,15aα)]- (9CI) (CA INDEX NAME)



RN 151341-78-5 HCAPLUS
CN L-Valine, N,N-dimethyl-, 3,4,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-4-oxo-2H-3,15a-epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-6-yl ester, [3R-(3a,5bα,6α,7aβ,13bα,13cβ,15aα)]-

L9 ANSWER 20 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



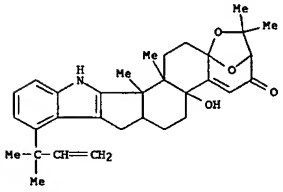
L9 ANSWER 21 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Jun 1994
ACCESSION NUMBER: 1994:291795 HCAPLUS
DOCUMENT NUMBER: 120:291795
TITLE: Tremorgenic Indole Alkaloids Potently Inhibit Smooth Muscle High-Conductance Calcium-Activated Potassium Channels
AUTHOR(S): Knaus, Hans-Guenther; McManus, Owen B.; Lee, Seok H.; Schmalhofer, William A.; Garcia-Calvo, Margarita; Helms, Lisa M. H.; Sanchez, Manuel; Giangiacomo, Kathleen; Reuben, John P.; et al.
CORPORATE SOURCE: Department of Membrane Biochemistry and Biophysics, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Biochemistry (1994), 33(19), 5819-28
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Tremorgenic indole alkaloids produce neurol. disorders (e.g., staggers syndromes) in ruminants. The mode of action of these fungal mycotoxins is not understood but may be related to their known effects on neurotransmitter release. To determine whether these effects could be due to inhibition of K+ channels, the interaction of various indole diterpenes with high-conductance Ca2+-activated K+ (maxi-K) channels was examined Paspalitrem A, paspalitrem C, aflatrem, penitrem A, and paspalinine inhibit binding of [125I]charybdotoxin (ChTX) to maxi-K channels in bovine aortic smooth muscle sarcolemmal membranes. In contrast, three structurally related compds., paxilline, verruculogen, and paspalicine, enhanced toxin binding. As predicted from the binding studies, covalent incorporation of [125I]ChTX into the 31-kDa subunit of the maxi-K channel was blocked by compds. that inhibit [125I]ChTX binding and enhanced by compds. that stimulate [125I]ChTX binding. Modulation of [125I]ChTX binding was due to allosteric mechanisms. Despite their different effects on binding of [125I]ChTX to maxi-K channels, all compds. potently inhibited maxi-K channels in electrophysiol. expts. Other types of voltage-dependent or Ca2+-activated K+ channels examined were not affected. Chemical modifications of paxilline indicate a defined structure-activity relationship for channel inhibition. Paspalicine, a dehydroxy analog of paspalinine lacking tremorgenic activity, also potently blocked maxi-K channels. Taken together, these data suggest that indole diterpenes are the most potent nonpeptidyl inhibitors of maxi-K channels identified to date. Some of their pharmacol. properties could be explained by inhibition of maxi-K channels, although tremorgenicity may be unrelated to channel block.

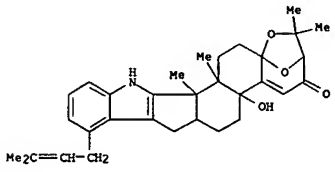
IT 11024-55-8, Paspalicine 63722-90-7, Paspalitrem A
63722-91-8, Paspalinine 70553-75-2, Aflatrem
90866-61-8, Paspalitrem C
RL: BIOL (Biological study)
(calcium-activated potassium channels of aorta smooth response to)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

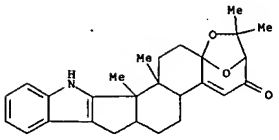
L9 ANSWER 21 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



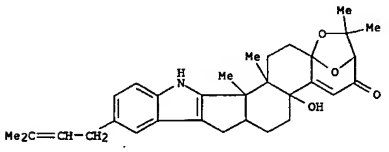
RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



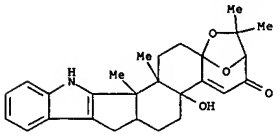
L9 ANSWER 21 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



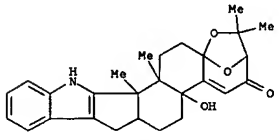
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 22 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:127325 HCAPLUS
DOCUMENT NUMBER: 120:127325
TITLE: Tremorgenic mycotoxins having indoloditerpene moiety
AUTHOR(S): Nozawa, Koohei
CORPORATE SOURCE: Fac. Pharm. Sci., Hoshi Univ., Tokyo, 142, Japan
SOURCE: Mycotoxins (1993), 37, 17-21
CODEN: MAIKD3; ISSN: 0285-1466
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Indoloditerpene moiety-containing tremorgenic mycotoxins were reviewed. The mass fragment of paxilline an its derivs. isolated from Emericella such as emindole SB paspaline, dehydroxypaxilline, and paxilline acetate were disclosed. The structures and biosynthetic pathways of other tremorgens isolated from Aspergillus flavus and Penicillium crustosum were also disclosed. These tremorgens are biosynthesized from tryptophan and geranylgeraniol with 3 types of cyclization, i.e., the nominine-, the emindol, and the paspaline-type. Emeniveol recently isolated from E. nivea may be categorized into the paspaline-type with addnl. reactions to produce penitrem, janthitrem, and lolitrem type compds.

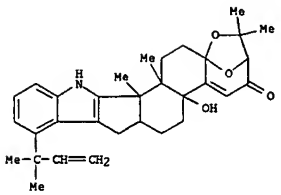
IT 63722-91-8, Paspalinine 70553-75-2, Aflatrem
RL: BIOL (Biological study)
(tremorgenic mycotoxin, indoloditerpene moiety-containing)

RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 22 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 23 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 25 Dec 1993

ACCESSION NUMBER: 1993:664674 HCAPLUS

DOCUMENT NUMBER: 119:264674

TITLE: Indole antiinsectan Aspergillus metabolites.

INVENTOR(S): Laakso, Jodi A.; Tepaske, Mark R.; Dowd, Patrick F.; Gloer, James B.; Wicklow, Donald T.; Staub, Gail M.

PATENT ASSIGNEE(S): United States Dept. of Agriculture, USA; University of Iowa Research Foundation; Biotechnology Research and Development Corp.

SOURCE: U.S., 12 pp. Cont.-in-part of U.S. 5,130,326.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5227396	A	19930713	US 1992-875360	19920429
US 5130326	A	19920714	US 1991-732786	19910719
US 5300495	A	19940405	US 1993-8616	19930122
WO 9322318	A1	19931111	WO 1993-US1834	19930226
W: AU, CA				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9337834	A	19931129	AU 1993-37834	19930226

PRIORITY APPLN. INFO.:

US 1991-732786	A2	19910719
US 1992-875360	A3	19920429
WO 1993-US1834	A	19930226

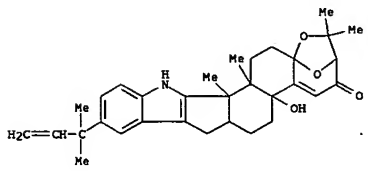
AB Sulpinine C, secopenitrem B and 10-oxo-11,33-dihydropenitrem B were isolated from the sclerotia of A. sulphureus. Aflatrem B was isolated from the sclerotia of A. flavus, and 14-hydroxypaspalinine and 14-(N,N-dimethylvalyloxy)paspalinine from the sclerotia A. nomius. The compds. control Coleoptera and Lepidoptera. Addition of 200 ppm aflatrem B to the diet of corn earworm (Helicoverpa zea) larvae, caused 57.2% weight reduction after 1 wk.

IT 144446-23-1, Aflatrem B 151341-77-4 151341-78-5
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(insecticide, from Aspergillus)

RN 144446-23-1 HCAPLUS

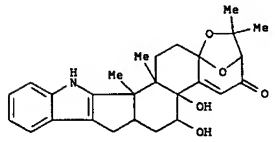
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 10-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3aα,5bα,7aβ,13b.alph a.,13cβ,15aα)-(+)- (9CI) (CA INDEX NAME)

L9 ANSWER 23 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



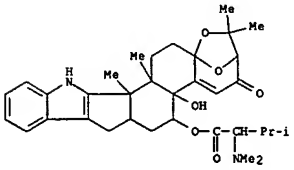
RN 151341-77-4 HCAPLUS

CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b,6-dihydroxy-2,2,13b,13c-tetramethyl-, [3R-(3α,5bα,6α,7aβ,13bα,13c.bet a.,15aα)]- (9CI) (CA INDEX NAME)



RN 151341-78-5 HCAPLUS

CN L-Valine, N,N-dimethyl-, 3,4,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-4-oxo-2H-3,15a-epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-6-yl ester, [3R-(3α,5bα,6α,7aβ,13bα,13cβ,15aα)]- (9CI) (CA INDEX NAME)



L9 ANSWER 24 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 30 Mar 1993

ACCESSION NUMBER: 1993:118970 HCAPLUS

DOCUMENT NUMBER: 118:118970

TITLE: Sulpinines, secopenitrem B and aflatrem B insecticidal metabolites from fungi

INVENTOR(S): Laakso, Jodi A.; TePaske, Mark R.; Dowd, Patrick F.; Gloer, James B.; Wicklow, Donald T.

PATENT ASSIGNEE(S): United States Dept. of Agriculture, USA; University of Iowa Research Foundation; Biotechnology Research and Development Corp.

SOURCE: U.S., 9 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

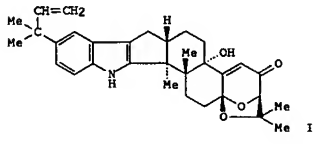
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5130326	A	19920714	US 1991-732786	19910719
US 5227396	A	19930713	US 1992-875360	19920429
WO 9301721	A1	19930204	WO 1992-US5956	19920716
W: AU, CA				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
AU 9223820	A	19930223	AU 1992-23820	19920716
US 5300495	A	19940405	US 1993-8616	19930122

PRIORITY APPLN. INFO.:

US 1991-732786	A2	19910719
US 1992-875360	A3	19920429
WO 1992-US5956	A	19920716

GI



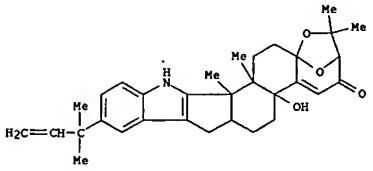
AB The indole derivs. sulpinines A, B, and C and secopenitrem B were isolated from Aspergillus sulphureus, and the new aflatrem B (I) from A. flavus. The above compds. are insecticides, especially against Coleoptera and Lepidoptera. A 57.2% reduction in weight gain of Helicovespa zea, relative to controls, was observed after 1 wk, when 200 ppm I was incorporated into the diet.

IT 144446-23-1, Aflatrem B
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(as insecticide, from Aspergillus flavus)

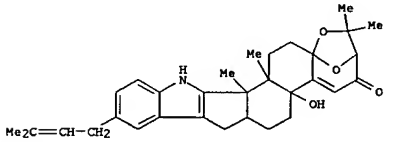
RN 144446-23-1 HCAPLUS

CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 10-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3aα,5bα,7aβ,13b.alph

L9 ANSWER 24 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
a.,13cβ,15aα)-(+)- (9CI) (CA INDEX NAME)

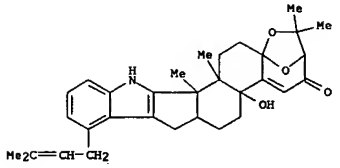


L9 ANSWER 25 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 03 Feb 1993
ACCESSION NUMBER: 1993:34196 HCAPLUS
DOCUMENT NUMBER: 118:34196
TITLE: Tremorgenic mycotoxins, paspalitrem A and C, from a tropical Phomopsis
AUTHOR(S): Bills, Gerald F.; Giacobbe, Robert A.; Lee, Seok H.; Pelaez, Fernando; Tkacz, Jan S.
CORPORATE SOURCE: Dep. Basic Microbiol., Merck Res. Lab., Rahway, NJ, 07065, USA
SOURCE: Mycological Research (1992), 96(11), 977-83
CODEN: MYCRER; ISSN: 0953-7562
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An endophytic Phomopsis species from living bark of Cavendishia pubescens in Colombia produced paspalitrem A and paspalitrem C in batch ferms. These compds. previously were known only from sclerotia of Claviceps paspali as tremorgenic mycotoxins causing neurol. disorders of livestock. A potential ecol. role of these metabolites in regard to endophytism of the woody host is considered.
IT 63722-90-7, Paspalitrem A 90866-61-8, Paspalitrem C
RL: BIOL (Biological study)
(of tropical Phomopsis, tremor from)
RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

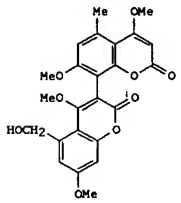


RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 25 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



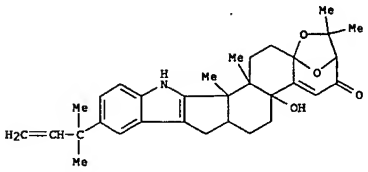
L9 ANSWER 26 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 13 Dec 1992
ACCESSION NUMBER: 1992:629702 HCAPLUS
DOCUMENT NUMBER: 117:229702
TITLE: Aflavarin and β-aflatrem: new anti-insectan metabolites from the sclerotia of Aspergillus flavus
AUTHOR(S): TePaske, Mark R.; Gloer, James B.; Wicklow, Donald T.; Dowd, Patrick F.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Journal of Natural Products (1992), 55(8), 1080-6
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



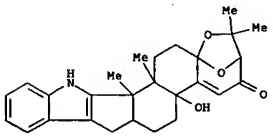
I

AB Aflavarin (I), a new bicoumarin, and β-aflatrem (II), an isomer of the tremorgen aflatrem, were isolated from the sclerotia of A. flavus. The structures were determined through a series of 1D and 2D NMR expts., assisted by spectral comparisons with known compds. I exhibits potent antifeedant activity against the fungivorous beetle Carpophilus hemipterus. II causes a significant reduction in the growth rate of the corn earworm Helicoverpa zea. The presence of nominine as a minor metabolite of A. flavus is reported for the 1st time.
IT 144446-23-1, β-Aflatrem
RL: BIOL (Biological study)
(insect inhibitor, from Aspergillus flavus)
RN 144446-23-1 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 10-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3α,5bα,7aβ,13b.alph a.,13cβ,15aα)-(+)- (9CI) (CA INDEX NAME)

L9 ANSWER 26 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

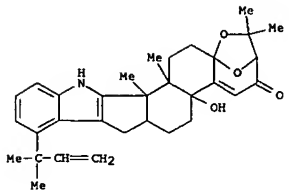


IT 63722-91-8, Paspalinine 70553-75-2, Aflatrem
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of Aspergillus flavus)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

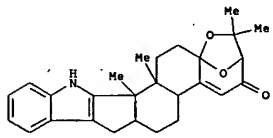


RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

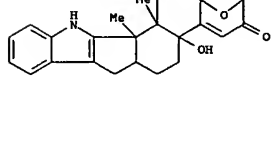
L9 ANSWER 26 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 27 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 03 Apr 1992
ACCESSION NUMBER: 1992:129335 HCAPLUS
DOCUMENT NUMBER: 116:129335
TITLE: Total syntheses of (+)-paspalicine and (+)-paspalinine
AUTHOR(S): Sunazuka, T.; Smith, A. B., III; Leenay, T. L.; Wood, J. K.
CORPORATE SOURCE: Res. Cent. Biol. Funct., Kitasato Inst., Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1991), 33rd, 172-9
CODEN: TYKYDS
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB A symposium on the total synthesis of the title compds. in which a unified strategy in synthesis of (-)-paspaline is exploited.
IT 11024-55-8P, (+)-Paspalicine 63722-91-8P, (+)-Paspalinine
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



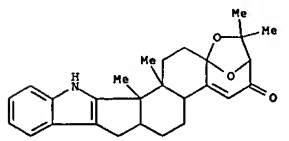
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 03 Apr 1992
ACCESSION NUMBER: 1992:129296 HCAPLUS
DOCUMENT NUMBER: 116:129296
TITLE: Indole diterpene synthetic studies. 8. The total synthesis of (+)-paspalicine and (+)-paspalinine
AUTHOR(S): Smith, Amos B., III; Kingery-Wood, Jill; Leenay, Tamara L.; Nolen, Ernest G.; Sunazuka, Toshiaki
CORPORATE SOURCE: Dep. Chem., Univ. Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Journal of the American Chemical Society (1992), 114(4), 1438-49
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:129296
GI

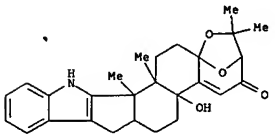
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The development of a unified synthetic strategy for the indole diterpene tremorgens has led to the first total syntheses of (+)-paspalicine (I; R = H) and (+)-paspalinine (I; R = OH), in 22 and 23 steps, resp. The cornerstone of the approach is the intermediacy of (-)-II this proposed common precursor to the simple indole diterpenes was previously generated in nine steps from (+)-Wieland-Miescher ketone (III) in an earlier synthesis of (-)-paspaline. Key transformations include installation of the indole unit via the Gassman protocol, alkylation of the thermodn. anion of dimethylhydrazone IV with epoxide (-)-V, and RhCl3-promoted isomerization of the β,γ-unsatd. ketone in (+)-VI to afford I (R = H). I (R = OH) in turn was secured via SeO2 oxidation of I (R = H), a particularly noteworthy result given the importance of the C(4b) hydroxyl group for tremorgenic activity. MM2 calcns. revealed that I embody the less stable relative configuration of the F- and G-ring bicyclic ketal moiety.
IT 138331-69-8 138331-70-1
RL: PRP (Properties)
(force-field calcns. of conformation of)
RN 138331-69-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, [3S-(3α,5bβ,7aα,13bβ,13cα,15aα)]- (9CI) (CA INDEX NAME)

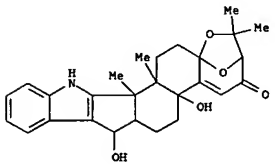


RN 138331-70-1 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one,

L9 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, [3S-(3α,5bβ,7aα,13bβ,13cα,15a.alpha.)]- (9CI) (CA INDEX NAME)

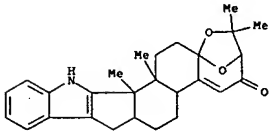


IT 138235-49-1P
RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in preparation of paspalicine)
RN 138235-49-1 HCAPLUS
CN 2H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4(3H)-one, 5b,6,7,7a,8,13,13b,13c,14,15-decahydro-5b,8-dihydroxy-2,2,13b,13c-tetramethyl- (9CI) (CA INDEX NAME)

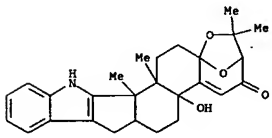


IT 63722-90-7P 63764-58-9P 90866-61-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthetic strategy for preparation of)
RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

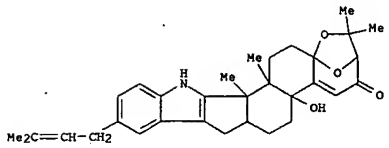
L9 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(+)-Paspalinine
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



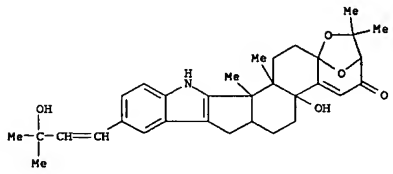
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



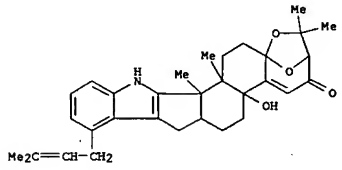
L9 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

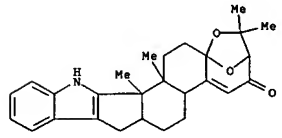


RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

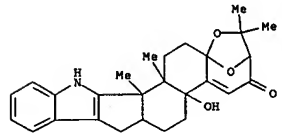


IT 11024-55-8P, (+)-Paspalicine 63722-91-8P,

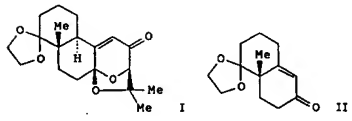
L9 ANSWER 29 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 27 Dec 1991
ACCESSION NUMBER: 1991:680346 HCAPLUS
DOCUMENT NUMBER: 115:280346
TITLE: The total synthesis of (+)-paspalicine and (+)-paspalinine
AUTHOR(S): Klingery-Wood, Jill Elizabeth
CORPORATE SOURCE: Univ. Pennsylvania, Philadelphia, PA, USA
SOURCE: (1991) 266 pp. Avail.: Univ. Microfilms Int., Order No. DA9125690
From: Diss. Abstr. Int. B 1991, 52(3), 1438-9
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 11024-55-8P, (+)-Paspalicine 63722-91-8P, (+)-Paspalinine
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 30 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Nov 1991
ACCESSION NUMBER: 1991:632568 HCAPLUS
DOCUMENT NUMBER: 115:232568
TITLE: Synthetic studies towards paspalicine: preliminary investigations, and the synthesis of 3',4',7',7'a,9',10',11',11'a-octahydro-4',4',7'a-trimethylspiro[1,3-dioxolane]-2,8'(6'H)-2'H-3',5'a-epoxynaphth[2,1-b]oxepin-2'-one
AUTHOR(S): Ali, Amin; Guile, Simon D.; Saxton, J. Edwin; Thornton-Pett, Mark
CORPORATE SOURCE: Sch. Chem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Tetrahedron (1991), 47(32), 6407-26
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:232568
GI

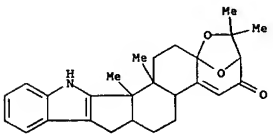


I II

AB An efficient route to the characteristic β-pyrone ketal functionality of paspalicine has resulted in the preparation of ketal I, containing the requisite stereochem., in 8 steps from the monoketal II of the Wieland-Miescher ketone in an overall yield of 8.0%.

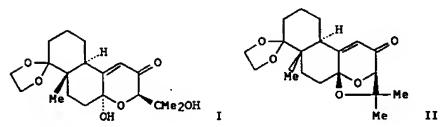
IT 11024-55-8, Paspalicine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of intermediates for)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 30 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L9 ANSWER 31 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Jun 1991
ACCESSION NUMBER: 1991:228600 HCAPLUS
DOCUMENT NUMBER: 114:228600
TITLE: Synthetic studies towards paspalicine. Part 2. Synthesis of the eastern half
AUTHOR(S): Guile, Simon; Saxton, J. Edwin; Thornton-Pett, Mark
CORPORATE SOURCE: Sch. Chem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Tetrahedron Letters (1991), 32(10), 1381-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

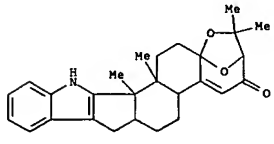


I II

AB Intramol. cyclocondensation of hydroxypropylnaphthopyranone I gave dioxolonaphthopyranone II. The crystal structure of I and II is reported.

IT 11024-55-8P, Paspalicine
RL: SPN (Synthetic preparation); PREP (Preparation)
(dioxolonaphthopyranone fragment of, stereoselective preparation of)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

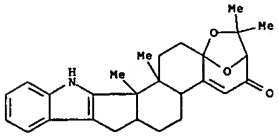


L9 ANSWER 32 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Jun 1991
ACCESSION NUMBER: 1991:222917 HCAPLUS
DOCUMENT NUMBER: 114:222917
TITLE: Isolation and determination of paspalitrem-type tremorgenic mycotoxins using liquid chromatography with diode-array detection
AUTHOR(S): Selala, M. I.; Musuku, A.; Schepens, P. J. C.
CORPORATE SOURCE: Toxicol. Cent., Univ. Antwerp, Wilrijk, 2610, Belg.
SOURCE: Analytica Chimica Acta (1991), 244(1), 1-8
CODEN: ACACAM; ISSN: 0003-2670
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A liquid chromatog. (LC) method is described for the isolation and determination of the tremorgenic mycotoxins paxilline (Penicillium paxilli NRRL 6110), paspaline, paspalinine, and paspalicine (Claviceps paspali). Following a Soxhlet extraction of a mold-contaminated matrix using chloroform, the crude extract was partitioned between hexane and 80% aqueous methanol. The latter fraction, containing the desired toxin(s), was evaporated to dryness, the residue dissolved in methylene chloride, and the solution analyzed by liquid chromatog. using a Supelcosil LC-Si column eluted with methylene chloride-di-Et ether (9 + 1, volume/volume). A mixture containing stds. of these compds. was similarly analyzed. All toxins were detected using a UV diode-array detector. The generated UV spectra and chromatog. data of the standard toxins were stored in a computer as a library and used to identify these toxins in a crude mixture The purity of the separated peaks and the amount of toxin in the crude mixture were also determined The toxins were isolated by selectively collecting the eluted peaks using a programmable fraction collector equipped with a peak level sensor. Further confirmation of compound identity was achieved by mass spectrometry using the direct inlet probe method. In comparison with methods used previously to isolate these toxins, the present technique is fast and allows the acquisition of complete UV spectral information and chromatog. data and the isolation of multiple toxins in a single chromatog. operation.

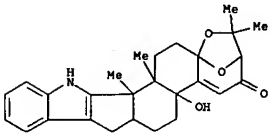
IT 11024-55-8, Paspalicine 63722-91-8, Paspalinine
RL: BIOL (Biological study)
(isolation and determination of, from Claviceps paspali by liquid chromatog. with diode-array detection)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

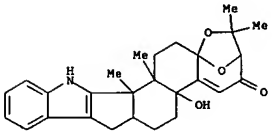


•L9 ANSWER 32 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



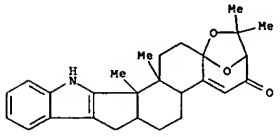
L9 ANSWER 33 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 33 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 May 1991
ACCESSION NUMBER: 1991:207536 HCAPLUS
DOCUMENT NUMBER: 114:207536
TITLE: Total syntheses of (+)-paspalicine and (+)-paspalinine
AUTHOR(S): Smith, Amos B., III; Sunazuka, Toshiaki; Leenay, Tamara L.; Kingery-Wood, Jill
CORPORATE SOURCE: Monell Chem. Senses Cent., Univ. Pennsylvania, Philadelphia, PA, 19104, USA
SOURCE: Journal of the American Chemical Society (1990), 112(22), 8197-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:207536
GI

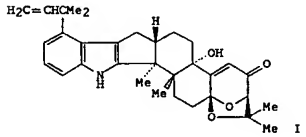
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Total syntheses of the indole diterpenes (+)-paspalicine (I) (R = H) (II) and paspalanine I (R = OH) were achieved in 22 and 23 steps, resp., via a unified strategy applicable to the entire class of simple indole tremorgens. The intermediacy of tricyclic ketone III prepared in 9 steps from (+)-Wieland-Miescher ketone, served as the starting material for this approach. Central features of the scheme included installation of the indole unit via the Gassman protocol, construction of rings F and G by alkylation of the thermodn. anion of the dimethylhydrazone of (+)-IV with epoxide (-)-V, and an RhCl3-promoted migration of the β,γ-olefinic bond in (+)-VI to afford II. (+)-Paspalinine in turn was secured via SeO2 oxidation of II. The latter transformation is important given the requirement of a C(4b) tertiary hydroxyl group for tremorgenic activity.
IT 11024-55-8P 63722-91-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



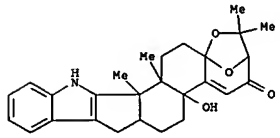
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-

L9 ANSWER 34 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 29 Sep 1990
ACCESSION NUMBER: 1990:510705 HCAPLUS
DOCUMENT NUMBER: 113:110705
TITLE: Production of alfatrem and its related indoloditerpenes by microsclerotium-producing strains of Aspergillus flavus
AUTHOR(S): Tanaka, T.; Hasegawa, A.; Aoki, N.; Yamamoto, S.; Udagawa, S.; Sekita, S.; Harada, M.; Nozawa, K.; Kawai, K.
CORPORATE SOURCE: Public Health Res. Inst., Kobe, 650, Japan
SOURCE: Mycotoxins (1989), 30, 19-23
CODEN: MAIKD3; ISSN: 0285-1466
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI



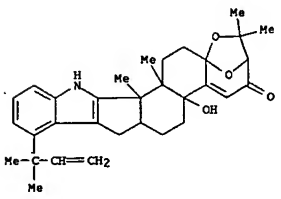
I

AB Four strains of atypical A. flavus isolated from Indonesian traditional medicines (native name, Jamu) and three representative strains of the same fungus obtained from the Northern Regional Research Center, USDA were cultured on Czapek-yeast extract agar at 34° and the amts. of the tremorgenic mycotoxins, aflatrem (I) and seven related indoloditerpenes, were measured by high-performance liquid chromatog. with a UV detector. All strains examined produced I and dihydroxyaflavinine. The concns. of them ranged from 149 to 3009 and 1092 to 35,629 μg/g of the dried sclerotia, resp. Aflavinine, monohydroxyaflavinine, monohydroxyisoaflavinine, paspaline, paspalinine, and emindole SB were detected in the sclerotia of A. flavus. This is the first report on the production of emindole SB and paspaline by A. flavus.
IT 63722-91-8, Paspalinine 70553-75-2, Aflatrem
RL: FORM (Formation, nonpreparative)
(formation of, by Aspergillus flavus)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

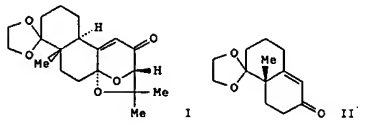


L9 ANSWER 34 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

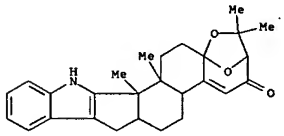
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



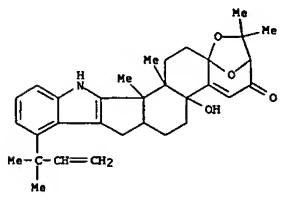
L9 ANSWER 35 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 Apr 1990
ACCESSION NUMBER: 1990:158678 HCAPLUS
DOCUMENT NUMBER: 112:158678
TITLE: Towards paspalicine: synthesis of rings D-G
AUTHOR(S): Ali, Amin; Saxton, J. Edwin
CORPORATE SOURCE: Sch. Chem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Tetrahedron Letters (1989), 30(24), 3197-200
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:158678
GI



AB The β-pyrone ketal I, which constitutes rings D-G of the mold metabolite paspalicine, was prepared in 50%, overall yield from the monoketal II.
IT 11024-55-8P, Paspalicine
RL: PREP (Preparation)
(synthesis of rings D-G of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

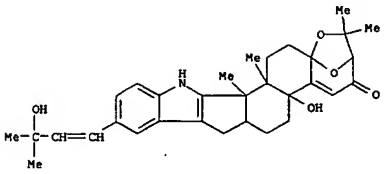


L9 ANSWER 36 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 Mar 1990
ACCESSION NUMBER: 1990:115080 HCAPLUS
DOCUMENT NUMBER: 112:115080
TITLE: Gradient high-performance liquid chromatography using alkylphenone retention indices of insectidical extracts of Penicillium strains
AUTHOR(S): Russell, R.; Paterson, M.; Kemmelmeier, Carlos
CORPORATE SOURCE: Int. Mycol. Inst., CAB, Kew/Surrey, TW9 3AF, UK
SOURCE: Journal of Chromatography (1989), 483, 153-68
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Purified exts. of 4 Penicillium strains which were active against the insect pest Spodoptera littoralis were analyzed by gradient HPLC for secondary metabolites using alkylphenone retention indexes. HPLC of pure secondary metabolite stds. detected previously in the exts. by TLC was undertaken in order to obtain bracketed retention indexes. More metabolites were detected by HPLC than by TLC, although some compds. detected by TLC in some strains were not detected by this HPLC method. A minority of metabolites were exclusive to each strain, and most were produced by >1 strain. The profiles were more characteristic of each strain when only the larger peaks were considered. This emphasizes the importance of detection limits in secondary metabolite anal. Some of the implications of these analyses to fungus toxicity and systematic mycol. are discussed.
IT 70553-75-2, Aflatrem
RL: PROC (Process)
(separation of, of Penicillium by HPLC)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

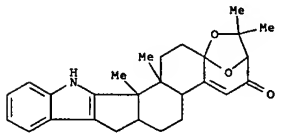


L9 ANSWER 37 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Dec 1989
ACCESSION NUMBER: 1989:628778 HCAPLUS
DOCUMENT NUMBER: 111:228778
TITLE: Experimental constraints in the study of the biosynthesis of indole alkaloids in fungi
AUTHOR(S): Laws, Ian; Mantle, Peter G.
CORPORATE SOURCE: Dep. Biochem., Imp. Coll. Sci., Technol. Med., London, SW7 2AY, UK
SOURCE: Journal of General Microbiology (1989), 135(10), 2679-92
CODEN: JGMIAN; ISSN: 0022-1287
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The disproportionate difficulty in obtaining compelling exptl. evidence from 14C-radiolabeling that the indole moiety of the otherwise isoprenoid penitrem A is biosynthesized by Penicillium crustosum directly from tryptophan was explored. [benzene ring-14C]Tryptophan added to the broth beneath the mycelial mat of stationary liquid cultures labeled penitrem A with 1.4% incorporation, only 3-fold more than that determined for [methylene-14C]tryptophan or [U-14C]tyrosine, incorporation of which could only have been indirect. In contrast, the substituted tryptophan-histidine diketopiperazine roquefortine, biosynthesized concurrently with penitrems by this organism, was labeled with compelling efficiency (23.4% incorporation of [benzene ring-14C]tryptophan). In submerged culture, Claviceps paspali concurrently biosynthesized an analogous pair of metabolites, 3-hydroxy-3-methylbutenyl paspalinine and lysergic acid α-hydroxyethylamide. This feature enabled the exptl. demonstration of [benzene ring-14C]tryptophan incorporation to an extent more consistent with direct contribution of the indole moiety of the indole-diterpenoid paspalinine derivative The same precursor applied to the sporing surface of P. crustosum stationary cultures also provided stronger evidence for a direct biosynthetic role in the formation of penitrem A. In the absence of competition from any other indolic secondary metabolite, a submerged culture of Penicillium paxilli incorporated 5% of the [benzene ring-14C]tryptophan given during growth into the indole-diterpenoid paxilline. A double-labeling time-course experiment indicated temporal separation of steps in the biosynthesis of roquefortine. The inadequacy of classical precursor techniques for studying biosynthesis of indole-diterpenoids in P. crustosum is discussed. The more homogeneous submerged culture fermentation system is preferred for experimentation.
IT 63764-58-9
RL: FORM (Formation, nonpreparative)
(formation of, from tryptophan by fungi, study of)
RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

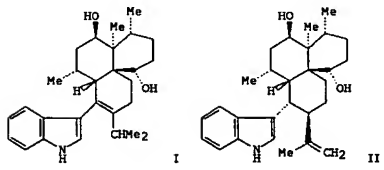
•L9 ANSWER 37 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



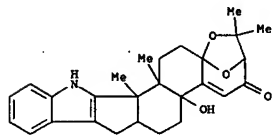
L9 ANSWER 38 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 Nov 1989
ACCESSION NUMBER: 1989:574479 HCAPLUS
DOCUMENT NUMBER: 111:174479
TITLE: The total synthesis of (-)-paspaline and progress toward the total synthesis of (+)-paspalicine
AUTHOR(S): Leenay, Tamara Leigh
CORPORATE SOURCE: Univ. Pennsylvania, Philadelphia, PA, USA
SOURCE: (1988) 273 pp. Avail.: Univ. Microfilms Int., Order No. DA8816198
From: Diss. Abstr. Int. B 1989, 49(7), 2652-3
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 11024-55-8P, (+)-Paspalicine
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



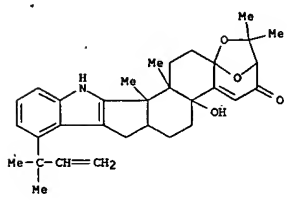
L9 ANSWER 39 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 01 Oct 1989
ACCESSION NUMBER: 1989:512074 HCAPLUS
DOCUMENT NUMBER: 111:112074
TITLE: Studies of fungal products. Part XXVI. Isolation and structures of two new indoloditerpenes related to aflavinine from a microsclerotium-producing strain of Aspergillus flavus
AUTHOR(S): Nozawa, Koohei; Sekita, Setsuko; Harada, Masatoshi; Udagawa, Shunichi; Kawai, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Hoshi Univ., Tokyo, 142, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1989), 37(3), 626-30
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



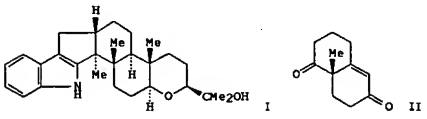
AB Along with paspalinine, aflatrem, alfavinine, and dihydroxyaflavinine, two new indoloditerpenes, monohydroxyaflavinine (I) and monohydroxyisoaflavinine (II), were isolated from the CH2C12 extract of a microsclerotium-producing strain of A. flavus, which has activity to produce aflatoxins. The structures of the above compds. were determined on the basis of spectroscopic investigations and x-ray crystal analyses of I acetone solvate and II.
IT 63722-91-8, Paspalinine 70553-75-2, Aflatrem
RL: BIOL (Biological study)
(from Aspergillus flavus)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 39 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

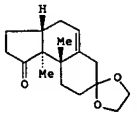


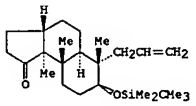
L9 ANSWER 40 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 20 Aug 1989
ACCESSION NUMBER: 1989:458121 HCAPLUS
DOCUMENT NUMBER: 111:58121
TITLE: Indole diterpene synthetic studies. 5. Development of a unified synthetic strategy; a stereocontrolled, second-generation synthesis of (-)-paspaline
AUTHOR(S): Smith, Amos B., III; Leenay, Tamara L.
CORPORATE SOURCE: Monell Chem. Senses Cent., Univ. Pennsylvania, Philadelphia, PA, 19104-2326, USA
SOURCE: Journal of the American Chemical Society (1989), 111(15), 5761-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:58121
GI



I

II

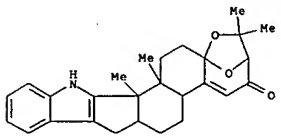

III



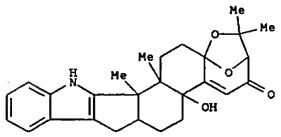
IV

AB A highly stereocontrolled, second-generation synthesis of (-)-paspaline (I) is described. The synthesis proceeded via an initial nine-step conversion of (+)-Wieland-Miescher ketone (II) to tricyclic cyclopentanone III, an intermediate that is expected to be useful for the construction of other members of this family of tremorgenic indole diterpene alkaloids. Completion of the synthetic scheme involved an eight-step transformation of III to the tricyclotridecanone IV, an advanced intermediate in the first total synthesis of I.
IT 11024-55-8, Paspalicine 63722-91-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(potential intermediate for, preparation of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 40 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

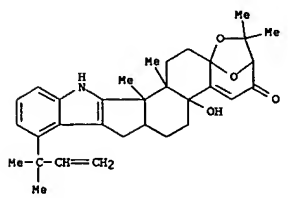


RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 41 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1989
ACCESSION NUMBER: 1989:167855 HCAPLUS
DOCUMENT NUMBER: 110:167855
TITLE: The tremorigen aflatrem is a positive allosteric modulator of the γ-aminobutyric acidA receptor channel expressed in Xenopus oocytes
AUTHOR(S): Yao, Y.; Peter, A. B.; Baur, R.; Sigel, E.
CORPORATE SOURCE: Dep. Pharmacol., Univ. Bern, Bern, CH-3010, Switz.
SOURCE: Molecular Pharmacology (1989), 35(3), 319-23
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Aflatrem potentiates the GABA-induced chloride current. This pos. allosteric regulatory action of aflatrem was quant. studied on the GABAA receptor channel expressed in Xenopus oocytes after injection with chick brain mRNA under voltage-clamp conditions. In this model system, aflatrem potentiates the current induced by 5 μM GABA in a concentration-dependent manner. Half-maximal potentiation was obtained with 2.4 μM aflatrem and maximal stimulation of the GABA (5 μM) response was more than 10-fold. The potentiation was not associated with a change of the reversal potential of the GABA-induced current. In the presence of 2 μM aflatrem, the GABA dose-response curve shifted to lower concns., with the Ka decreasing from 28 to 7 μM and the Hill coefficient, n, from 1.5 to 0.8, as measured at a membrane potential -100 mV. At saturating concentration of GABA (250 μM), aflatrem (10 μM) was still able to enhance the current by .apprx.21%. Further expts. suggest that the site of action of aflatrem on the GABAA receptor channel complex is different from that of benzodiazepines, pentobarbital, and picrotoxin. Aflatrem (10 μM) had no effect on the coexpressed voltage-dependent sodium and calcium channels and on the kainate channel. The potentiating action of aflatrem on the GABAA receptor channel may explain the initial symptoms of intoxication caused by aflatrem in vivo, i.e., diminished activity or immobility of the affected animal.
IT 70553-75-2, Aflatrem
RL: BIOL (Biological study)
(GABAergicA receptors of chloride channel of Xenopus oocyte response to)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

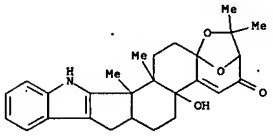


L9 ANSWER 41 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L9 ANSWER 42 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 11 Jun 1988
ACCESSION NUMBER: 1988:204858 HCAPLUS
DOCUMENT NUMBER: 108:204858
TITLE: Carbon-13 NMR spectroscopy of indole derivatives
AUTHOR(S): Morales-Rios, M. S.; Espineira, J.; Joseph-Nathan, P.
CORPORATE SOURCE: Cent. Invest. Estud. Avanzados, Inst. Politec. Nac., Mexico City, 07000, Mex.
SOURCE: Magnetic Resonance in Chemistry (1987), 25(5), 377-95
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The chemical shifts of 298 naturally occurring and synthetic compds. containing the indole chromophoric group are listed. Substituent effects on 13C chemical shifts (SCS) induced by substitution on the heteroarom. five-membered ring are discussed. The data provide a reference set for future 13C NMR investigations and highlight the need for unambiguous exptl. evidence to resolve controversial assignments for differently substituted representative indole derivs. Many original assignments have been changed, and values not considered to be unambiguously assigned are delineated. The 1J(CH) values for the parent indole were measured.

IT 63722-91-8, Paspalinine
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbon-13 NMR chemical shifts of)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

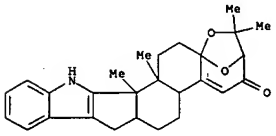


L9 ANSWER 43 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 01 Apr 1988
ACCESSION NUMBER: 1988:109279 HCAPLUS
DOCUMENT NUMBER: 108:109279
TITLE: Novel indoloditerpenes, emindoles, and their related compounds from Emericella spp
AUTHOR(S): Nozawa, Kohei; Nakajima, Seiichi; Kawai, Kenichi; Udagawa, Shunichi; Horie, Yoshikazu; Yamazaki, Mikio
CORPORATE SOURCE: Fac. Pharm. Sci., Hoshi Univ., Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1987), 29, 637-43
CODEN: TYKYDS
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

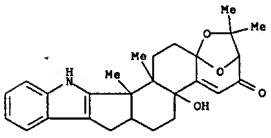
AB In the course of survey of paxilline (I) in Emericella spp., new-type indoloditerpenes, emindoles DA (II) and DB (III), and emindole SA (IV), were isolated from the mycelial extract of E. desertorum and E. striata, resp. The structure of II, III, and IV were determined on the basis of the spectroscopic and chemical data of their derivs. and x-ray crystallog. of emindole DA monoacetate. Three new compds. related to I, emindole SB, dehydroxypaxilline, and paxilline acetate, were also isolated along with I and paspaline from the mycelium of E. striata, and their structures were elucidated by the spectroscopic and chemical investigation. Two different types of indoloditerpenes, emindole SA and paxilline analogs (paspaline, emindole SB, dehydroxypaxilline, and paxilline acetate) were isolated from the same fungus, E. striata. Isolation of paspaline, emindole SB, dehydroxypaxilline and paxilline acetate from the same fungus may suggest the biogenesis of I.

IT 11024-55-8P 63722-91-8P 70553-75-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

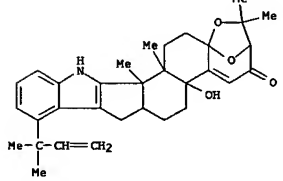


RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one,

L9 ANSWER 43 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



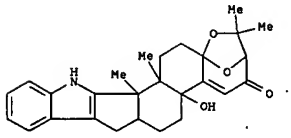
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 44 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 Dec 1987
ACCESSION NUMBER: 1987:613332 HCAPLUS
DOCUMENT NUMBER: 107:213332
TITLE: Action of tremorgenic mycotoxins on GABAA receptor
AUTHOR(S): Gant, Daniel B.; Cole, Richard J.; Valdes, James J.; Eldefrawi, Mohyee E.; Eldefrawi, Amira T.
CORPORATE SOURCE: Sch. Med., Univ. Maryland, Baltimore, MD, 21201, USA
SOURCE: Life Sciences (1987), 41(19), 2207-14
CODEN: LIFSAK; ISSN: 0024-3205
DOCUMENT TYPE: Journal
LANGUAGE: English

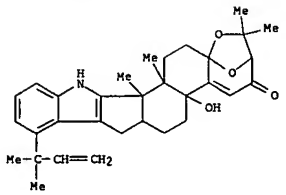
AB The effects of 4 tremorgenic and 1 nontremorgenic mycotoxins were studied on γ-GABAA receptor binding and function in rat brain and on binding of a voltage-operated Cl- channel in Torpedo elec. organ. None of the mycotoxins had significant effect on [3H]muscimol or [3H]flunitrazepam binding to the GABAA receptor. However, only the 4 tremorgenic mycotoxins inhibited GABA-induced 36Cl- influx and [35S]-tert-butylbicyclophosphorothionate ([35S]TBPS) binding in rat brain membranes, while the nontremorgenic verruculotoxin had no effect. Inhibition of [35S]TBPS binding by paspalinine was noncompetitive. This suggests that tremorgenic mycotoxins inhibit GABAA receptor function by binding close to the receptor's Cl- channel. On the voltage-operated Cl- channel, only high concns. of verruculogen and verruculotoxin caused significant inhibition of the channel's binding of [35S]TBPS. The tremorgenic action of these mycotoxins may be due in part to their inhibition of GABAA receptor function.

IT 63722-91-8, Paspalinine 70553-75-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(GABA receptors of brain response to)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 44 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 45 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 27 Nov 1987

ACCESSION NUMBER: 1987:592376 HCAPLUS

DOCUMENT NUMBER: 107:192376

TITLE: Standardized high-performance liquid chromatography of 182 mycotoxins and other fungal metabolites based on alkylphenone retention indexes and UV-VIS spectra (diode array detection)

AUTHOR(S): Frisvad, Jens; Thrane, Ulf

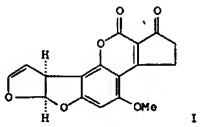
CORPORATE SOURCE: Dep. Biotechnol., Tech. Univ. Denmark, Lyngby, DK-2800, Den.

SOURCE: Journal of Chromatography (1987), 404(1), 195-214
CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

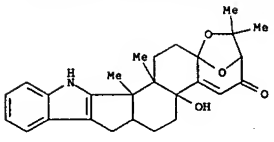
AB A general standardized method for the anal. of mycotoxins and other fungal secondary metabolites was developed, based on HPLC with an alkylphenone retention index and photodiode-array detection combined with TLC in 2 different eluents. Each fungal secondary metabolite is characterized by its bracketed alkylphenone retention time index, its UV-VIS absorption maximum and its retardation factors relative to griseofulvin in 2 TLC eluents. This system is effective for the comparison of chemotaxonomic data in different labs. and for a precise identification of fungi based on organic solvent exts. of fungal cultures. All important groups of mycotoxins and other fungal secondary metabolites could be detected in the HPLC system described and data are listed for 182 metabolites. The fungal secondary metabolites separated and characterized include aflatoxin B1 (I), B2, G1 and G2, ochratoxin A, citrinin, penicillin acid, viomellein, penitrem A, patulin, sterigmatocystin, alternariol, tenuazonic acid, trichothecenes, roquefortines, fusarin C, zearalenone, PR-toxin, citreoviridin, viridicatumtoxin, verruculogen, rugulosin, cyclopiazonic acid, penicillin G, and many other alkaloids, polyketides, and terpenes.

IT 63722-91-8, Paspalinin 70553-75-2, Aflatrem
RL: ANT (Analyte); ANST (Analytical study)
(HPLC and TLC determination of)

RN 63722-91-8 HCAPLUS

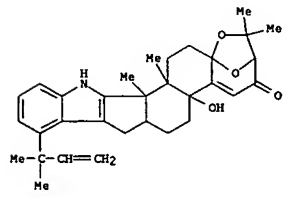
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 45 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 70553-75-2 HCAPLUS

CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 46 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 14 Nov 1987

ACCESSION NUMBER: 1987:570268 HCAPLUS

DOCUMENT NUMBER: 107:170268

TITLE: Dihydropyridine receptors: possible allosteric regulation by tremorgenic toxins

AUTHOR(S): Valdes, J. J.; Wolff, V. L.; Ross, D. H.

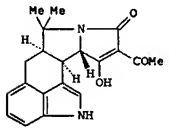
CORPORATE SOURCE: Health Sci. Cent., Univ. Texas, San Antonio, TX, USA

SOURCE: Report (1986), CRDEC-TR-87008; Order No. AD-A175458/9/GAR, 16 pp. Avail.: NTIS
From: Gov. Rep. Announce. Index (U. S.) 1987, 87(7), Abstr. No. 712,405

DOCUMENT TYPE: Report

LANGUAGE: English

GI



I

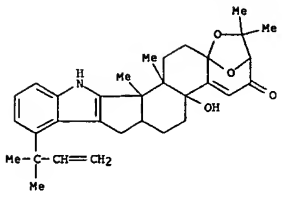
AB Dihydropyridine (DHP) receptors appear to be coupled to voltage-sensitive Ca channels that mediate Ca2+ flux in neural tissue. A number of toxins known to interact with these channels induce tremors and seizures and modulate the ability of DHP compds. to alter the gating properties of Ca2+ channels. It is therefore likely that tremorgenic mycotoxins may modulate Ca2+ channels either directly or by their ability to act at DHP receptors. Tremorgenic doses of aflatrem, cyclopiazonic acid (I), and verruculogen increase the number and decrease the affinity of DHP receptors in rat cortex. Presumably the Ca2+ channel and its associated receptors are important targets for several classes of fungal toxins.

IT 70553-75-2, Aflatrem
RL: BIOL (Biological study)
(dihydropyridine receptors of brain cortex response to calcium channels in relation to)

RN 70553-75-2 HCAPLUS

CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 46 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



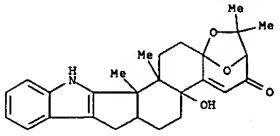
L9 ANSWER 47 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 08 Aug 1987
ACCESSION NUMBER: 1987:436247 HCAPLUS
DOCUMENT NUMBER: 107:36247
TITLE: High-performance liquid chromatographic determination of profiles of mycotoxins and other secondary metabolites
AUTHOR(S): Frisvad, Jens C.
CORPORATE SOURCE: Dep. Biotechnol. Food Technol., Tech. Univ. Denmark, Lyngby, DK-2800, Den.
SOURCE: Journal of Chromatography (1987), 392, 333-47
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A reversed-phase HPLC determination of profiles of mycotoxins and other fungal secondary metabolites was developed. Penicillium, Aspergillus, And Fusarium polyketides, terpenes, and alkaloids were emphasized. In a gradient elution, using H2O-MeCN containing 0.05% CF3COOH, 134 secondary metabolites were eluted evenly with retention times of 1.08-34.48 min. Metabolites with the same retention time were usually not produced by the same species. As UV detection at 254 nm was used, some mycotoxins (type A trichothecenes, viridicatumtoxin, peptide-like compds., and xanthomegnin) could not be detected. The method appears to be valuable for chemotaxonomic studies of fungi. Unpurified concentrated CHCl3-MeOH exts. of petri dish cultures analyzed by the proposed method presented gave species-specific characteristic profiles of known and unknown secondary metabolites and mycotoxins.

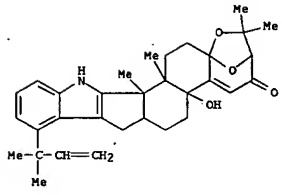
IT 63722-91-8, Paspalinin 70553-75-2, Aflatrem
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, from fungi)

RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 47 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



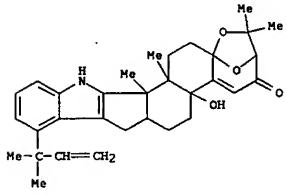
L9 ANSWER 48 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 26 Dec 1986
ACCESSION NUMBER: 1986:620582 HCAPLUS
DOCUMENT NUMBER: 105:220582
TITLE: The potent tremorgenic neurotoxins lolitrem B and aflatrem: a comparison of the tremor response in mice
AUTHOR(S): Gallagher, R. T.; Hawkes, A. D.
CORPORATE SOURCE: Ruakura Anim. Res. Stn., Ministr. Agric. Fish., Hamilton, N. Z.
SOURCE: Experientia (1986), 42(7), 823-5
CODEN: EXPEAM; ISSN: 0014-4754
DOCUMENT TYPE: Journal
LANGUAGE: English

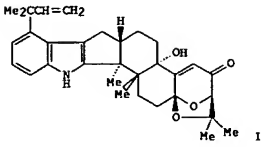
AB Tremor dose-response curves were determined for mice dosed with the ryegrass neurotoxin lolitrem B (I) [81771-19-9] and the tremorgenic mycotoxin aflatrem [70553-75-2]. A family of characteristic curves was revealed for each tremorgen, with I eliciting a sustained tremor response persisting for >24 h.

IT 70553-75-2
RL: BIOL (Biological study)
(tremor from, lolitrem B in relation to)

RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 49 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Apr 1986
ACCESSION NUMBER: 1986:124633 HCAPLUS
DOCUMENT NUMBER: 104:124633
TITLE: Aflatrem: a tremorgenic mycotoxin with acute neurotoxic effects
AUTHOR(S): Valdes, James J.; Cameron, Jacqueline E.; Cole, Richard J.
CORPORATE SOURCE: Toxicol. Div., Chem. Res. Dev. Cent., Aberdeen Proving Ground, MD, 21010-5423, USA
SOURCE: Environmental Health Perspectives (1985), 62, 459-63
CODEN: EVHPA2; ISSN: 0091-6765
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



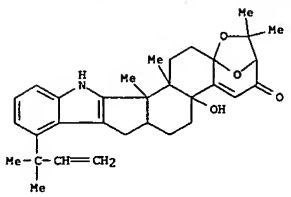
I

AB Rats were given a single tremorgenic (3 mg/kg, i.p.) dose of aflatrem (I) [70553-75-2], and kinetics of amino acid neurotransmitter uptake was assessed in isolated hippocampal nerve terminals at 1 day, 1 wk, and 2 wk after injection. Results indicate a decrease in the capacity of the GABA [56-12-2] and glutamate [56-86-0] uptake systems, which was interpreted as a loss of nerve terminals. The affinity consts. suggest a decrease in release of these transmitters as well. In addition to its transient influence on transmitter release, a single low dose of I is able to induce degeneration of neuronal processes in hippocampal neurotransmitter systems and therefore represents a long-term health threat.

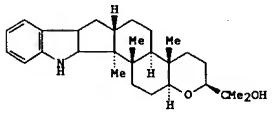
IT 70553-75-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(neurotransmitter uptake by hippocampus synaptosome response to)

RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 49 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 50 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 13 Oct 1984
ACCESSION NUMBER: 1984:526410 HCAPLUS
DOCUMENT NUMBER: 101:126410
TITLE: Paspalitrem C, a new metabolite from sclerotia of Claviceps paspali
AUTHOR(S): Dorner, Joe W.; Cole, Richard J.; Cox, Richard H.; Cunfer, Barry M.
CORPORATE SOURCE: Natl. Peanut Res. Lab., U.S. Dep. Agric., Dawson, GA, 31742, USA
SOURCE: Journal of Agricultural and Food Chemistry (1984), 32(5), 1069-71
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

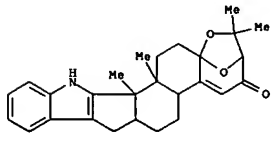


I

AB A new metabolite was purified from CHCl3 exts. of C. paspali sclerotia by column chromatog. and preparative, centrifugally accelerated TLC. The chemical structure of the metabolite was determined by 1H- and 13C-NMR spectroscopy to be paspalitrem C (I). Paspalitrem C differed from the previously identified tremorgen, paspalitrem A, only by the position of attachment of the 3-methyl-2-butenyl unit to the indole ring.

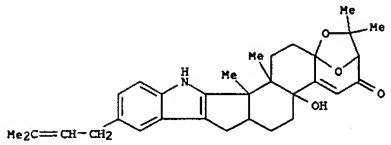
IT 11024-55-8 63722-90-7 63722-91-8
63764-58-9
RL: BIOL (Biological study)
(from Claviceps paspali)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

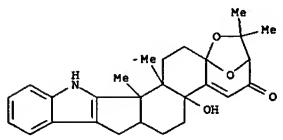


RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

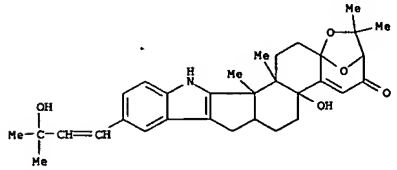
L9 ANSWER 50 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



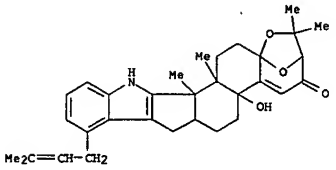
RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



IT 90866-61-8
RL: BIOL (Biological study)
(of Claviceps paspali, separation and structure of)

RN 90866-61-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-9-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

L9 ANSWER 50 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

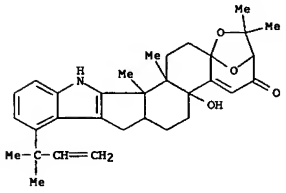


L9 ANSWER 51 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1982:468963 HCAPLUS
DOCUMENT NUMBER: 97:68963
TITLE: Tremorgenic indole metabolites and aflatoxins in sclerotia of Aspergillus flavus: an evolutionary perspective
AUTHOR(S): Wicklow, Donald T.; Cole, Richard J.
CORPORATE SOURCE: North. Reg. Res. Cent., Sci. Educ. Adm., Peoria, IL, 61604, USA
SOURCE: Canadian Journal of Botany (1982), 60(5), 525-8
CODEN: CJBOAW; ISSN: 0008-4026
DOCUMENT TYPE: Journal
LANGUAGE: English

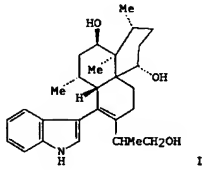
AB Isolates of A. flavus from both cool and warm latitudes were cultured on potato dextrose agar containing yeast extract to identify sclerotia-producing strains. CHCl3-MeOH exts. of sclerotia were analyzed for the presence of aflatoxins and major indole metabolites (e.g., cyclopiazonic acid, aflatrem, and dihydroxyaflavinine). Aflatoxin is reported from sclerotia of A. flavus for the 1st time. Cyclopiazonic acid was detected primarily in sclerotia of isolates from warmer latitudes. Aflatrem and dihydroxyaflavinine were detected in sclerotia from 85% of the strains examined These metabolites are associated with the sclerotial stage of the life cycle, because neither were detected in exts. of the culture medium and mycelium of Petri dish cultures from which all the sclerotia were removed. Geog. variation and intrafungal allocation of these toxic compds. in A. flavus are examined from the evolutionary ecologist's perspective of selective forces shaping the chemical defense systems of fungi.

IT 70553-75-2
RL: BIOL (Biological study)
(of Aspergillus flavus sclerotia, evolution in relation to)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

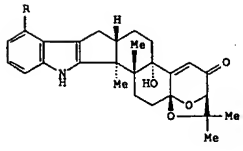


L9 ANSWER 52 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1981:135636 HCAPLUS
DOCUMENT NUMBER: 94:135636
TITLE: Indole metabolites from a strain of Aspergillus flavus
AUTHOR(S): Cole, Richard J.; Dorner, Joe W.; Springer, James P.; Cox, Richard H.
CORPORATE SOURCE: Natl. Peanut Res. Lab., Sci. Educ. Adm., Dawson, GA, 31742, USA
SOURCE: Journal of Agricultural and Food Chemistry (1981), 29(2), 293-5
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

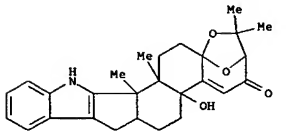


II, R=CMe2C:CH2
III, R=H

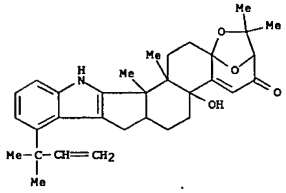
AB The x-ray structure of dihydroxyaflavinine (I), a new diterpene indole metabolite from A. flavus is reported. The fungal tremorgens aflatrem (II) and paspalinine (III) were also isolated from the A. flavus isolate. Previously, paspalinine had been reported from sclerotia of Claviceps paspali.

IT 63722-91-8 70553-75-2
RL: BIOL (Biological study)
(from Aspergillus flavus)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

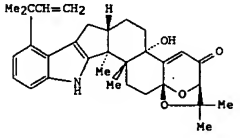
L9 ANSWER 52 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

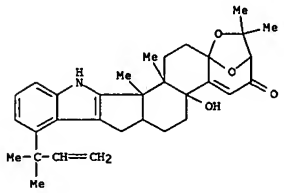


L9 ANSWER 53 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1980:446902 HCAPLUS
DOCUMENT NUMBER: 93:46902
TITLE: Aflatrem, a tremorgenic toxin from Aspergillus flavus
AUTHOR(S): Gallagher, Rex T.; Clardy, Jon; Wilson, Benjamin J.
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA
SOURCE: Tetrahedron Letters (1980), 21(3), 239-42
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

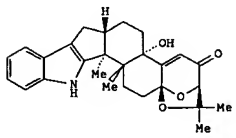


I

AB The mol. structure of aflatrem (I) was determined by UV, IR, 13C NMR, and mass
spectroscopy. The structure is very similar to that of paspalinine, a tremorgen from Claviceps paspali.
IT 70553-75-2P
RL: PREP (Preparation)
(from Claviceps paspali, structure of)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

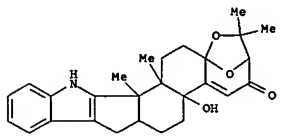


L9 ANSWER 54 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1980:446901 HCAPLUS
DOCUMENT NUMBER: 93:46901
TITLE: Paspalinine, a tremorgenic metabolite from Claviceps paspali Stevens et Hall
AUTHOR(S): Gallagher, Rex T.; Finer, Janet; Clardy, Jon; Leutwiler, Albert; Weibel, Franz; Acklin, Werner; Arigoni, Duilio
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA
SOURCE: Tetrahedron Letters (1980), 21(3), 235-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

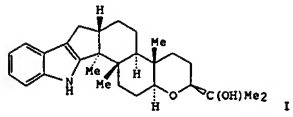


I

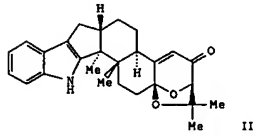
AB The structure and absolute configuration of paspalinine (I) were determined by UV,
IR, and NMR spectroscopy, and by x-ray crystallog.
IT 63722-91-8P
RL: PREP (Preparation)
(from Claviceps paspali, structure and absolute configuration of)
RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 55 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1980:446900 HCAPLUS
DOCUMENT NUMBER: 93:46900
TITLE: Paspaline and paspalicine, two indole-mevalonate metabolites from Claviceps paspali
AUTHOR(S): Springer, James P.; Clardy, Jon
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA
SOURCE: Tetrahedron Letters (1980), 21(3), 231-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

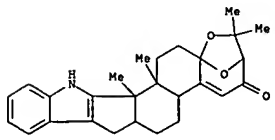


I

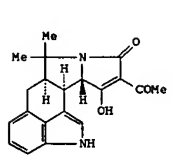


II

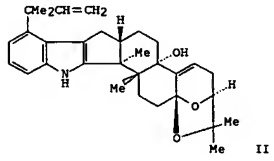
AB Crystal and mol. structures are presented for paspaline (I) and paspalicine (II).
IT 11024-55-0P
RL: PREP (Preparation)
(from Claviceps paspali, crystal structure of)
RN 11024-55-0 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 56 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1979:589416 HCAPLUS
DOCUMENT NUMBER: 91:189416
TITLE: Multiple toxin production by an isolate of Aspergillus flavus
AUTHOR(S): Richard, J. L.; Gallagher, R. T.
CORPORATE SOURCE: Natl. Anim. Dis. Cent., Sci. Educ. Adm., Ames, IA, 50010, USA
SOURCE: Mycopathologia (1979), 67(3), 161-3
CODEN: MYCPAH; ISSN: 0369-299X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

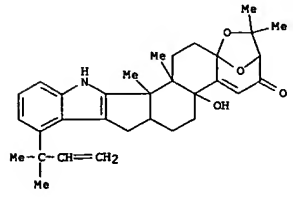


I



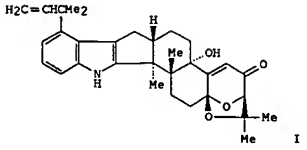
II

AB Three toxins were recovered from rice and wheat cultures of an isolate of A. flavus. The toxins were present simultaneously in the cultures after 1 or 2 wk incubation and were identified as aflatoxin, cyclopiazonic acid (I), and aflatrem (II), a recently identified indole-mevalonate metabolite.
IT 70553-75-2
RL: FORM (Formation, nonpreparative)
(formation of, by Aspergillus flavus)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



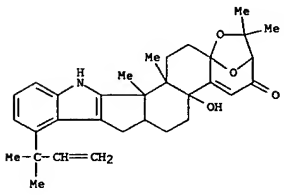
L9 ANSWER 56 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L9 ANSWER 57 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1979:433550 HCAPLUS
DOCUMENT NUMBER: 91:33550
TITLE: Aflatrem, the tremorgenic mycotoxin from Aspergillus flavus
AUTHOR(S): Gallagher, Rex T.; Wilson, Benjamin J.
CORPORATE SOURCE: Appl. Biochem. Div., Dep. Sci. Ind. Res., Palmerston North, N. Z.
SOURCE: Mycopathologia (1979), 66(3), 183-5
CODEN: MYCPAH; ISSN: 0369-299X
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
GI



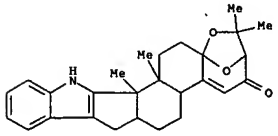
I

AB A review and discussion with 15 refs. on tremorgenic aflatrem (I) [70553-75-2] from A. flavus.
IT 70553-75-2
RL: BIOL (Biological study)
(of Aspergillus aflavus)
RN 70553-75-2 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 9-(1,1-dimethyl-2-propenyl)-2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

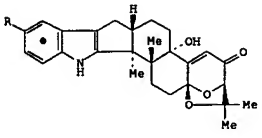


L9 ANSWER 57 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L9 ANSWER 58 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1978:402054 HCAPLUS
DOCUMENT NUMBER: 89:2054
TITLE: Structural studies of naturally occurring toxicogenic compounds
AUTHOR(S): Springer, J. P.
CORPORATE SOURCE: Ames Lab., Ames, IA, USA
SOURCE: Report (1977), IS-T-757, 107 pp. Avail.: NTIS
From: Energy Res. Abstr. 1978, 3(7), Abstr. No. 15917
DOCUMENT TYPE: Report
LANGUAGE: English
AB The paralytic shellfish poison, saxitoxin, is a neurotoxin isolated from Alaska butter clams (Saxidomus giganteus), mussels (Mytilus californianus), and axenic cultures of the dinoflagellate, Gonyaulax catenella. The structure of saxitoxin was determined by single crystal x-ray diffraction. It possessed a unqiue tricyclic arrangement of atoms containing 2 guanidinium moieties and a hydrated ketone. The relative stereochem. is presented as well as the absolute configuration. The chemical constitution of a tremorgenic metabolite, paxilline, isolated from exts. of the fungus, Penicillium paxilli, was also determined Paxilline represents a previously unreported class of natural compds. formed by the combination of tryptophan and mevalonate subunits. The complete stereostructure of 2 other fungal metabolites. paspaline and paspalicine, closely related to paxilline but isolated from Claviceps paspali were also determined The stereochem. of paxilline, paspaline, and paspalicine are identical at corresponding chiral centers.
IT 11024-55-8
RL: PROC (Process)
(structure study of)
RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



L9 ANSWER 59 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1978:46068 HCAPLUS
DOCUMENT NUMBER: 88:46068
TITLE: Paspalum staggers: isolation and identification of tremorgenic metabolites from sclerotia of Claviceps paspali
AUTHOR(S): Cole, Richard J.; Dorner, Joe W.; Lansden, John A.; Cox, Richard H.; Pape, Countney; Cunfer, Barry; Nicholson, Stephen S.; Bedell, David M.
CORPORATE SOURCE: Natl. Peanut Res. Lab., Dawson, GA, USA
SOURCE: Journal of Agricultural and Food Chemistry (1977), 25(5), 1197-201
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



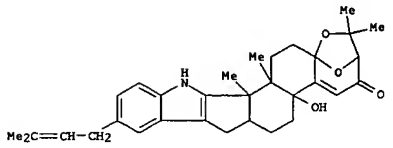
I, R=H
II, R=$CH_2CH{=}CMe_2$
III, R=$CH{=}CHCMe_2OH$

AB The neurol. disorder, Dallisgrass poisoning or paspalum staggers, occurs in cattle that graze Paspalum dilatatum infected with the fungus C. paspali and occurs sporadically in the southern portions of the U.S. Three tremorgenic metabolites were isolated from C. paspali sclerotia collected from P. dilatatum, and identified by spectroscopic methods. One of the metabolites identical with paspalinine (I), a previously reported metabolite of C. paspali. The remaining 2 metabolites differ from I in that they contain an addnl. isoprene and hydroxyisoprene unit attached to carbon 6 of the 6-membered indole ring, and are 3-methyl-2-butenylpaspalinine (II) and 3-hydroxy-3-methyl-1-butenylpaspalinine (III), resp.

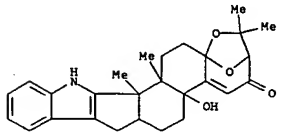
IT 63722-90-7 63722-91-8 63764-58-9
RL: PROC (Process)
(isolation of, from Claviceps paspali)

RN 63722-90-7 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-10-(3-methyl-2-butenyl)-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

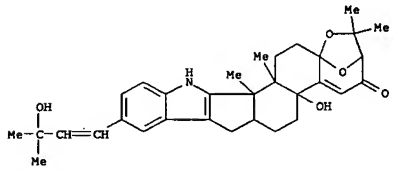
L9 ANSWER 59 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 63722-91-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)



RN 63764-58-9 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-5b-hydroxy-10-[(1E)-3-hydroxy-3-methyl-1-butenyl]-2,2,13b,13c-tetramethyl-, (3R,5bS,7aS,13bS,13cR,15aS)- (9CI) (CA INDEX NAME)

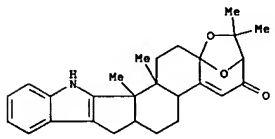


L9 ANSWER 60 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1975:564398 HCAPLUS
DOCUMENT NUMBER: 83:164398
TITLE: Structure of paxilline, a tremorgenic metabolite of Penicillium paxilli
AUTHOR(S): Springer, James P.; Clardy, Jon; Wells, John M.; Cole, Richard J.; Kirksey, Jerry W.
CORPORATE SOURCE: Dep. Chem., Iowa State Univ., Ames, IA, USA
SOURCE: Tetrahedron Letters (1975), (30), 2531-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB Crystals of paxilline (I) were orthorhombic, space group P212121, with a 31.009, b 11.522, and c 7.707 Å; R was 0.04 from 1840 observed reflections. The CD spectrum of I showed pos. Cotton effects for the first 2 bands and a neg. Cotton effect for a third band.

IT 11024-55-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure for paspalicine)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)

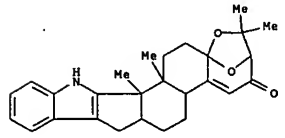


L9 ANSWER 61 OF 61 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 12 May 1984
ACCESSION NUMBER: 1967:479 HCAPLUS
DOCUMENT NUMBER: 66:479
TITLE: Isolation of 2 new indole derivatives from the mycelia of Claviceps paspali
AUTHOR(S): Fehr, Th.; Acklin, Werner
CORPORATE SOURCE: Tech. Hochsch., Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1966), 49(6), 1907-10
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German

AB C. paspali mycelia were extracted with pentane, Et2O, CHCl3, or CHCl3-MeOH (2:1, satd. with NH3), and the exts. were separated on a kieselgel G column. Fractions were studied by thin-layer chromatography using kieselgel HF. Indole derivs. were detected with the van Urk reagent (Groeger and Erge, CA 60, 367a), green spots with indoles. Rf values for CHCl3 were: 0.7 paspalicin (I), 0.35 paspalin (II), and 0.3 and 0.2 for unknowns. I, C31H35O4N, m. 230° (decomposition) (MeOH), [α]D = 173° (c 0.5), is a disubstituted indole with 4 tertiary methyls and 1 α,β-unsatd. carbonyl structure. II, C28H39O2N, m. 264° [α]D = -23° (c 0.36), is a 2,3-disubstituted indole derivative, and contains 5 tertiary methyls, 1 OH, and 1 ether-type O, and has a 1.7% yield. Acetylation of II gave an O-Ac derivative, m. 196° (hexane, sublimation), [α]D = -17° (c 0.66). The mevalonate origin of II was demonstrated with mevalonate-2-14C.

IT 11024-55-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 11024-55-8 HCAPLUS
CN 4H-3,15a-Epoxy-1-benzoxepino[6',7':6,7]indeno[1,2-b]indol-4-one, 2,3,5b,6,7,7a,8,13,13b,13c,14,15-dodecahydro-2,2,13b,13c-tetramethyl-, (3R,5bR,7aS,13bS,13cS,15aS)- (9CI) (CA INDEX NAME)



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=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	354.57	712.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-46.02	-46.02

STN INTERNATIONAL LOGOFF AT 17:49:23 ON 11 JAN 2007